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The workshops and the preparation of the reports have received funding from the European Union’s Horizon 2020 research and innovation programme under Grant Agreement No 723867
1. Executive summary

1.1 Description of the workshop and objectives

The rapid evolution of current technologies requires continuous development of improved materials in a wide range of industrial sectors. In this view, materials modelling techniques have the potential to serve as valuable and powerful means to accelerate industrial innovation. For this reason, the European Commission, through the European Materials Modelling Council, is strongly committed to promote the uptake of materials modelling by the European industry. To this goal, networking and collaboration among the different European stakeholders involved in the materials development sector – e.g. academic model developers, software owners, Translators (consultants) and end users – is to be promoted. Improved collaboration helps to identify critical areas needing development, possible bottlenecks for the adoption and use of materials models and to design proper strategies for more efficient exploitation and further development of materials models.

The objective of this meeting is therefore to gather a consistent number of experts (around 70) from the different stakeholders interested/involved in materials development and provide a discussion platform for industrial requirements as compared to state-of-the-art modelling techniques. The ambition of the workshop is to cover the more relevant aspects which are critical to the widespread adoption of materials modelling techniques in industry. To this, six thematic sessions are organized and will cover: 1) state-of-the-art modelling techniques and guidelines for further model developments; 2) the perspective of the European software owners/developers; 3) the economic impact of materials modelling on industrial innovation; 4) strategies for improving the two-way transfer of knowledge between academia and industry – i.e. Translators and their training requirements; 5) interoperability requirements and frameworks – e.g. ontologies – for integration of models and software. Finally, a special session will be dedicated to the discussion of the potential of artificial intelligence in the framework of materials modelling, with particular emphasis on the benefit for high-throughput simulations, big data and their mining – e.g. data-driven modelling – and industrial automation towards Industry 4.0.

In order to enhance the participation of the audience to the workshop, at the end of each session some questions were posed from the session chair to the audience in the form of an interactive poll, to which the attendees could give an answer using the laptop or mobile phone.

A dedicated website has been set-up on the EMMC website with information on the meeting:

https://emmc.info/events/emmc-torino2019/

Where the scheduled sessions and speakers were reported together with ancillary information on travelling, accommodation and participation details.
1.2 Major outcome

A total of 66 experts confirmed participation to the meeting, while only 3 were not finally present at the event. The participation was divided by industry, academy and Research Technology Office (RTO) as follows:

The participation type chart on the left demonstrates a good balance among all the stakeholders involved in materials modelling activities. Participating countries were: Austria, Sweden, Italy, UK, Germany, Norway, France, Ireland, Poland, Netherlands, Denmark, US, Spain, Slovenia, Belgium.

A total of 21 invited speakers were present (19 from EU and 2 from US) over six thematic sessions. The meeting took place at Politecnico di Torino (Italy) on 8-10 July 2019. The flyer of the meeting and the header designed for the event are reported below.

While the meeting was planned as an invitation-only event, the last special Session 6 about Artificial Intelligence and Industry 4.0 was left open to participation from the public (being this session an additional one and not originally planned in the framework of the formal EMMC-CSA activities).

The meeting was advertised (for information and for the open Session 6) on social networks of the EMMC and also via the press office of Politecnico di Torino:

http://www.politocomunica.polito.it/events/appuntamenti/(idnews)/13352

Finally, some collective pictures taken at the meeting are reported below.
2. Report of the meeting (main activities)

2.1 Welcome & introduction

Welcome address by POLITO: Roberto Zanino, Deputy Rector for EU relations

Politecnico di Torino is the oldest Technical University in Italy, established in 1859. Politecnico offers several courses in the field of Engineering, Architecture and Industrial Design to more than 35,000 students, including more than 600 PhD students. In 2019, the QS World University Ranking has ranked Politecnico di Torino at the 3rd place in the World for the Graduate Employment Rate. In order to make a continuous impact on a rapidly changing society, Politecnico di Torino developed a new Strategic Plan, which aims to address the most relevant challenges of our times. Among them, the digital transformation as a way to foster industrial production is one of the most important. Digital transformation of European industry presents enormous potential for growth in Europe, and the European Commission is putting effort into promoting advanced digital technologies in many industrial sectors. This workshop finds its placement in this framework. Materials modelling is a key part of the digital transformation and has the potential to serve as valuable and powerful tool to accelerate industrial innovation. Innovation requires the active role of all stakeholders and it is remarkable that industries, research technology organizations and academia attending this event are almost equally represented.

Welcome address by EMMC: Nadja Adamovic, Chair of the EMMC

The introductory presentation on the EMMC activities addressed the following points:

- General EMMC structure and how to participate
- The CSA project: coordinating, promoting actions, meetings and networking
- EMMC website, outreach activities, events and contributions to EC activities
2.2 Session 1: Materials modelling techniques

This session was organized in the framework of the activities of EMMC-CSA Working group “Model Development and Validation”, and chaired by Kersti Hermansson (Uppsala University, Sweden). The minutes of the invited talks (see also the abstract of the talks included in the program in the appendix), related discussions and instant polls for this session are reported below.

2.2.1 Report of the talks and related discussion

Elisa Molinari - University of Modena and Reggio Emilia (Italy)

Designing materials with HPC: the MaX European Centre

- **What MAX** is → European Centers of Excellence for HPC
  Vision of the HPC center is to introduce the discovery of materials codes and predicting property codes into the industry, as happened in fluid dynamics. Quantum mechanics + multiscale approach.
  MAX center: there are already 5 big HPC centers in Europe (JULIC, CINECA, …). They are the most important both for their HPC infrastructure and for their knowhow, and capabilities.
  Technical challenges: we expect a big change transition in hardware and drivers when we move towards and beyond exascale transition. Disruptive change. Codes and software should and must align with this huge transition.

  **Euro HPC:**
  - **funds:** 28 participants. Budget up to 2020: 1.4 Beuro. 2027 → 2.7 Beuro
  - **JOINT PROCUREMENT:** top machines for Europe. 3 pre-exascale and 5petascale sites
  - Research and Innovation

- **MAX:** focus of modelling materials and material simulations. Special effort on quantum material simulations.
  Open source software: Yambo, CP2K, Siesta, Fleur, Aiida Materials Cloud, quantum espresso…

- **Success Cases:**
  1) Code for friction and tribology calculation. Using QE and Aiida, they have been able to relate friction and lubrication to the electronic charge distribution. Breathing bands due to molecular order in CH3NH3Pbl3 M. Wierzbowska, J. J. Meléndez, D. Varsano
2) Substitution of artificial colorants with natural colorants: the first step was to simulate color. Simulation of the spectrum by considering molecules solvated

- Max offers: Consulting, training, support…
- See: http://www.max-centre.eu/

Arnulf Latz - German Aerospace Center (Germany)

Spatially resolved modeling and simulation of degradation in Lithium ion batteries

Germany aerospace center. EXZELLENT (HIU): Center of Excellence for research in electrochemical energy storage. Founded in Jan 2011. Computational Electrochemistry at DLR/HIU.
https://www.dlr.de/dlr//en/desktopdefault.aspx/tabid-10002/

- DEGRADATION: how can we model the dynamics of local degradation? Degradation depends on the interfacial phenomena between electrolytes and battery. SEI formation (solid electrolyte interface) and Lithium Plating properties: overpotential due to dissipative transport

Base model → Best: the aim of the model was to test and see what kind of structure is able to remain stable
Example (1): NMC (binder, carbon, black, NMC) and Graphite. What are the properties of such materials during the process of charge and discharge. cell voltage vs the depth of discharge.

Vladimir Lobaskin - University College Dublin (Ireland)

Multiscale modelling of bionano interface

Multi-scale modelling of bio-nano interface. H2020 project: SmartNanoTOx – NanoCommons – NanoSolvent. All these projects involve the interfaces/interaction between organic and inorganic materials. In few years a lot of developments in nanomedicine: therapy, drug delivery. But what happens at the nanolayer of such materials? Nanoparticle toxicity

Review of nanotoxicity: https://www.nature.com/articles/nnano.2012.207

What material properties determine their functionality, toxicity of biocompatibility.
- How does the material affect the processes in biotechnology?
- How can we improve drug delivery?
- How can we avoid fouling?
- Materials by design

There are several challenges to answer to these questions: lack of force field, lack of information, different time scales. We can split the problem into two parts: 1) physical understanding, 2) experimental data driven modelling. They have been combined to reach results and be predictive. Strategy: modelling protein (sequence of amico acids, 3D structure, ITAPPER software) and NP simultaneously (Descriptors). Put together the information to couple the modelling with the experimental data.

CG model of Protein Corona:

(2) NP (can be split in core and surface),

(3) study of adsorption of protein and NP, CG model of both. BONES methodology to study the force field developments. Orientational sampling of protein binding NPs


Ilian Todorov - Science and Technology Facilities Council (UK)

DL_MESO: The UK’s DPD Vehicle for Academic and Industrial Collaboration

Hartree Center:
Developer of DL_POLY: in order to deal with meso scale modelling, they added the software

DL_MESO: www.ccp5.ac.uk/DL_MESO : Within the ccp5 European initiative

MPI domain-decomposed codes: DPD and LBE.

In 2009 UK Gov invests for engineering (IBM)

In 2010 KCMC establishes computer aided formulation a venture between Unilever GSJ

In 2012 STFC and Unilever sign MoU for strategic

CAF ambition

Example (1): Simulation of CMC and phase diagram

2.2.2 Results of the polls and related discussion

The first question that was posed to the audience was: What does industry need from a MM point of view? The ranking of the provided options resulted as follows:

- generate ready-to-go solutions for identified challenges – 3.8 out of 5
- better evidence that MM can be an added value – 3.5 out of 5
- push data-driven solutions (artificial intelligence) – 3.3 out of 5
- advancing individual model types (continuum and discrete) – 3.2 out of 5
- advancing C&L methods and scale bridging – 3.2 out of 5
- more computational power (in-house / exascale) – 3.2 out of 5
It emerges that ready-to-go solutions are highly desirable, together with better documentation that materials modelling techniques provides benefit for industrial innovation (success stories). Also, data-driven solutions seem to be quite relevant, as they quite high among the proposed options.

Next question was to rate according to effort vs potential impact the model types development and that of C&L of models. Results are as follows (sorted by highest impact):

<table>
<thead>
<tr>
<th>Choices</th>
<th>Effort</th>
<th>Impact</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuum models</td>
<td>5.0</td>
<td>8.2</td>
</tr>
<tr>
<td>Mesoscopic models</td>
<td>6.3</td>
<td>6.6</td>
</tr>
<tr>
<td>C&amp;L of models</td>
<td>6.3</td>
<td>6.0</td>
</tr>
<tr>
<td>Atomistic models</td>
<td>6.6</td>
<td>5.8</td>
</tr>
<tr>
<td>Electronic models</td>
<td>7.8</td>
<td>5.4</td>
</tr>
</tbody>
</table>
It emerges that the highest impact is assigned to the adoption/development of continuum models, which are also those requiring less effort – likely being a more mature technology in industry. Mesoscopic models follow in terms of impact and similar effort. C&L is considered important, as well as atomistic models, yet still very challenging. Finally, from an industrial perspective, electronic models are considered very difficult to deploy/develop and relatively low-ranked in terms of potential impact. It is important to remark that these results are specific to the audience at the meeting and do not pretend to be exhaustive. For example, some attendees argued that, based on other collected feedback, electronic models are, at least, as relevant as atomistic and mesoscopic models from a software to industry perspective.

The third question was: C&L of models: does industry need it and why? This was left as open questions and the collected answer are reported in the next figure.

All the provided answers are reported below:

- Yes. But we need to provide case studies and value demonstration.
- Needs to reach the relevant time/length scales
- Yes, industry needs it but only where the lack of it prevents the development of significant products/services
- Extend scales to industrially-relevant ones
- We are still working out whether we need to. We certainly need modelling at the different scales, and there are applications where (for instance) transport and intrinsic kinetics are on similar timescales (+transient heat transfer is required)
- Yes, to understand the physics of materials.
- It is an effective way to provide lost cost, good accuracy models. News a lot of experts
- Coupling and linking can help to use the atomistic and molecular modelling results at macroscale and will help the validation of results
If your product development depends on multiscale aspect yes.
If not, black box might be sufficient (single scale)
Yes, optimization and searching solutions
Yes - There is a gap to be bridged
Industry needs it, as some complex problems cannot be solved on one scale or with one model.
Yes, the potential possibilities of these models are huge
Obviously, it would be good to have, however there is too much emphasis on it.
Coupling models, in the strong sense, introduces potential causes for incoherence and risks making results even worse; moreover, great efforts for development and maintenance are needed.
Simple linking (e.g., store results in a DB) is a necessity
Yes, but direct coupling usually does not worth.
Many individual models exist. Each is easier to develop, within a single expertise group. Coupling and linking is the most efficient way to enhance the usage.
Interoperability and reduce the "from idea to the market" time
Yes, for curing and storing results of the simulations
Real problems are intrinsically multidisciplinary, involving not only materials modelling but also environment, manufacturing, circular economy and economy
Yes, to optimize and improve physics of materials.
It's very important but it needs to improve in terms of reliability of results and in terms of the need for computational power vs usefulness of output produced
incorporate some microscopic understanding into meso and continuum models
Yes, to make models more transferrable, reliable, and efficient. In general, to apply them to a broader spectrum of challenges
Models are needed not only for their predictive capabilities, but also to rationalize the experimental evidence collected in industry
C&L is needed as more sophisticated materials depend on different scales and coupling gives a more accurate and better understanding of the overall dynamic performance
C&L has an associated cost beyond the linked scales' methodologies. Each solution is unique (no general purpose) hence the cost is high. Hence this is a high risk, high return, limited longevity, limited applicability task for industry.
It is important from a research point of view but not for industry
Definitely yes. Different scales need different approaches, but they should be compatible
Yes, but only when cost and accuracy of such models are worth it
Videogames can make good simulation so why can't we

Trying to summarize the emerging trends, C&L of models are generally considered to be important from an industrial perspective mainly to extend scales to industrially-relevant ones, even though special care should be taken about error propagation.
Finally, the last question was: How to increase industry’s trust in MM? Replies were:

<table>
<thead>
<tr>
<th>Choices</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benchmarks for verification &amp; validation of models</td>
<td>4.55</td>
</tr>
<tr>
<td>More accurate materials models and techniques</td>
<td>3.725</td>
</tr>
<tr>
<td>Advance uncertainty quantification (UQ) methods</td>
<td>3.55</td>
</tr>
</tbody>
</table>

Particular importance in this sense emerges for V&V benchmarks, which is considered a critical aspect to increase the trust and awareness of the potential of materials modelling in industry. On the other hand, UQ methods and techniques and better models are considered less important with regards to this specific question.

2.3 **Session 2: Software deployment**

This session was organized in the framework of the activities of EMMC-CSA Working Group “Industrial Software Deployment”, and chaired by Volker Eyert (Materials Design, France). Particularly, this session was included in the workshop as the Expert Group Meeting on “Cloud-based solutions” organized by the same group. The minutes of the invited talks (see also the abstract of the talks included in the program in the appendix), related discussions, and instant polls for this session are reported below.

2.3.1 **Report of the talks and related discussion**

**Beatrice Carasi - COMSOL (Italy)**

*Standard and advanced material modelling with COMSOL Multiphysics*

B. Carasi introduced COMSOL as easy to use and well-integrated software that can describe complex material behavior. COMSOL is asking industry what functionality they want to see in the software. Recognizable trends are thermal management and production and harvesting of energies. Industry generally has to follow norms and wants to see these in software as well. The future trends move towards additive manufacturing, the digital twin concept and the internet of things. When asked why COMSOL is so successful three main reasons where given: (i) support, (ii) integration and (iii) robustness. It is pertinent to listen to users but also to apply good customer
expectation management, as a Software owner can never cover all wishes. Software providers need to listen to the customer attentively and understand the end-users' needs in order to improve the code or develop new features for industrial software applications. Thus, the business of a software owner should be driven by the market's needs. Software releases with new features are seen as a good to have and COMSOL aims for 1-2 releases/annum, hence, the company comes across as very responsive to users, who always would like to see new things. COMSOL’s main income stems from developing and selling software; they offer support and training for the use of the software but no contract research. However, there is a network of 3rd party providers who could take the latter on.

**Umberto Martinez - Synopsys (Denmark)**  
*Lean and agile software development of the QuantumATK platform*

U. Martinez described agile methods as SCRUM as a preferred way to manage software development. Besides using SCRUM as a good framework for code development, Synopsys aims development to be driven by their customers and to reach maximum yield without sacrificing quality. Especially, the iteration cycles in agile development allow them fast implementation of new features and permits regular feedback. The risk of failing with new development is lowered and one can react faster and correct mistakes as they happen. The final product should be easy to deploy, i.e. it should come with a simple installer and good documentation. The customer-driven approach allows to collect feedback from the end-users and thereby to open new perspectives for code development. Synopsys' software is not black-box style and thus requires some user knowledge of modelling and the underlying theories. Synopsys provides support for industrial end-users in form of training and tutorials. Code developers contact engineers and manufacturing specialists of the customers to design user-friendly software for industrial applications. Developers working at Synopsys are mostly scientists (physicists), who gain knowledge in IT development by daily exposure to the agile development framework. The roles in an agile development team (usually 4-6 members), such as the SCRUM master, are rotated. Thus, each individual can learn management skills. The team members get confronted with user stories and have to assign the tests and reviews that come with them. The specific, individual expertise of each specialist gained during the development cycle is documented and archived. Code documentation prevents knowledge loss if employees move on; all has to be written down and knowledge can be recovered if needed. There is no trend for employees to design self-generated long-term projects – input for these are driven by EU research projects. However, the company evaluates the projects ideas, designs the project strategy and decides the project benefits for the company (possible realisation) based on the input from customers and own estimation. QuantumWise did merge with Synopsys and it is still very early in this new venture, but from the employees’ perspective the two cultures seem to work well.

**Gabriele Mogni (standing in for Timur Bazhirov) - Exabyte.io (US)**  
*Cloud computing for Materials Modeling*

G. Mogni started out listing several usage modes of cloud computing for materials ranging from users, who work on the level of applications, to users, who only want to take advantage of the infrastructure provided by the cloud. In general, the cloud can be public or private and could be managed even by a 3rd party provider. The technology is available for some time already, however, the public is not yet ready to embrace it. This was and still is due to a lot of inhibitors such as IP, safety, and license issues as well as the fact that workflows developed for HPC environments are not easily transferable to cloud computing. At the same time, cloud computing offers a lot of
advantages, as 1. making in-house HPC hardware infrastructure obsolete to a large part since the calculations are done in the cloud and the end user needs to have only a web browser, which allows access even from a smart phone, 2. the general accessibility of the cloud by all (allowed) end users of a company, which makes the cloud a highly collaborative ecosystem, 3. the reduced cost as compared to in-house hardware, 4. the flexibility of choosing service level and licensing schemes, and 5. the freedom from buying software licenses. In addition, according to the speaker, cloud computing is ideally suited for materials modelling as data transfer is usually very little. If a calculation can be done on 10-20 nodes it is particularly suited for cloud computing. In addition, materials modeling calculations often require high throughput and the cloud would offer virtually no waiting time (queues don’t really exist). Yet, in the discussion after the talk it was also mentioned that most of these criteria are also met by in-house HPC environments. As a downside of cloud computing the speaker mentioned the fact that storage of user data may not be transparent, i.e. it may not be clear where the user data are stored. Furthermore, IP issues still need to be clarified in case commercial software and commercial applications are to be run in the cloud. Needless to mention that data security and safety issues are extremely important for industrial end users of cloud computing.

2.3.2 Results of the polls and related discussion

The first question was: To ease uptake of MM software in industry, please rank the provided options. The results were as follows:

<table>
<thead>
<tr>
<th>Choices</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>successful case studies</td>
<td>29.5</td>
</tr>
<tr>
<td>flexibility of licensing schemes</td>
<td>21.0</td>
</tr>
<tr>
<td>software validation benchmarks</td>
<td>18.4</td>
</tr>
<tr>
<td>flexibility of training tools</td>
<td>17.3</td>
</tr>
<tr>
<td>cloud-based deployment and services</td>
<td>13.8</td>
</tr>
</tbody>
</table>
Case studies are considered the most important to ease the uptake of MM in industry. Flexibility of licensing schemes is also considered quite important from a software deployment point of view. A clear trend emerges about the smaller importance that is given to cloud solutions to increase the uptake of technical software for MM in industry. More specific question on this latter point will be presented next.

The next question was about desktop solutions vs cloud: In 3-5 years, industrial end users will tend to prefer...

The result is as follows.

Cloud-based solutions - 49%
In-house solutions - 51%

The audience is equally divided between the two options.

The next question was: What are the bottlenecks that restrict widespread use of cloud-based solutions? The raw results are as follows.

- IP security
- Security
- Ip
- Security.
- Security
- Security concerns
- Security
- Data Security
- Security reasons.
- Privacy and security
- Security
- Confidentiality of the data.
- Data leaves
• complex - is it not just easier to work on a single computing facility?
• security, licensing
• Trust and IP issues
• Privacy
• IP
• Confidentiality and security
• Cost vs advantages
• Mainly offered outside Europe
• Security
• The security
• Security
• Provider experience and quality of service, especially when using open stack solutions...
• Legal issues
• Privacy/security
• Need for extra training
• Cost and security
• There is a large barrier to get started. Getting people on board, cost, security, licenses, platform, integration to broader digital transformation, data analytics
• Reaching potential users, not wary of existing solutions
• How do I know that the software I want to use, will run on the hardware assigned to me in the cloud?
• Licensing
• IP
• Fest of bad security"
• Google is already offering demanding videogames on cloud
• Legacy license systems
• not flexible to customize
• It is like using a rental car vs my own
• payment models, splitting across business units and projects
• Licensing
• Corporate IT, they don’t always understand R&D
A clear trend about an issue with security and data protection emerges from the responses of the audience. This seems to represent actually the main bottleneck which may prevent large adoption of cloud-based solutions.

Finally, the last question: From a security perspective, which one do you trust more? Gave insight on what is the most trusted solution as of today in terms of software solutions.

### 2.4 Session 3: Economic impact of materials modelling

This session was organized in the framework of the activities of EMMC-CSA Working Group “Industrial Integration and Economic Impact”, and chaired by Donna Dykeman (ANSYS, UK). Particularly, this session was included in the meeting as the "Tactics for enterprises" (Focused workshop organized by the same group).
2.4.1 Report of the talks and related discussion

Glenn Jones - Johnson Matthey (UK)

Economic Impact of Materials Modelling in R&D: There is clearly value, but we are still some way from a quantitative measure

- Presentation of Johnson Matthey: specialty in chemical and sustainable technologies, in the field of clean air, efficient natural resources, health and new markets (batteries, fuel cells, catalysts), and they use modelling in all these sectors
- Presentation of the R&D structure and strategy in Johnson Matthey
- Different modelling techniques according to the state of development of the technology; from core science and applied R&D, to product development (CFD, thermodynamics, system modelling)
- Over the last decades there were a number of false starts for modelling (e.g. late 80s early 90s, due to overselling of codes). Moore's law + code development allows today to achieve more impact with modelling. But there is an implicit assumption that doing modelling provides a positive economic impact to the company: we should demonstrate it.
- We should care about economic impact of modelling to have business resources from the company (internal) and also from the government (external)
- Modelling leads to faster (maybe), better (probably), different (yes) solutions in R&D respect to pure experimental approach
- Patents: typically, no 100% in-silico driven patent. Simulations are integrated in broader projects leading to patents. However, simulations provide additional knowledge to support a patent application (e.g. new material for battery)
- Modelling can be also useful to interact with customers, to improve the credibility (e.g. with articles on scientific journals), demonstrate technological leadership, produce marketing material
- Modelling also improves the skills and depth of understanding of the staff, augmenting their typical empirical approach to R&D and bringing to new ideas
- Prioritizing research: fast turnaround to achieve stories to tell, longer applied projects dedicated to mature technologies, long term projects in collaboration with academics (curiosity-driven)
- HPC resources are fundamental: from hardware to cloud. Codes are fundamental: from electronic to continuum
- Indicators of modelling success: projects, papers, patents, business units using modelling, perceived value → success stories
- Quantitative analysis of modelling impact is not easy, since it is related to many other parts of R&D (e.g. tests, characterization, scale-up, …), which have different time scales
- If we deconvolute the modelling impact from other aspects in his company: ROI is typically = 8; approx. 5% of sales spent on R&D (a smaller part spent on modelling); creation of proprietary modelling repository
- In conclusion, materials modelling clearly provides value, they use "soft" descriptors to quantify it, but "hard" descriptors are still far to be identified

Emilio Paolucci - Politecnico di Torino (Italy)

University – Industry Collaboration in an innovative context: A discussion of inhibitors and enablers

- Academia-industry standard approach is a linear model: R&D then development, but this has a lot of issues; currently, it is better to have a non-linear approach, with academia more involved in all the stages to receive earlier feedbacks
- Complexity of collaboration is increasing (info asymmetries and skills gap); TRL advancement is largely underestimated (overcome TRL 6 is most difficult one, because is between academia and company and no one is willing to pay), EU is not investing enough in this; contrasting targets: papers vs. competitiveness
- The EMMC case: support the discussion between academia and industry in the specific field of materials modelling
- EMMC did a questionnaire on that: 273 respondents between academia, SME and large companies
- 10 barriers have been identified against materials modelling: technical inhibitors, communication inhibitors, economic inhibitors and relational inhibitors
- Guidelines for action to overcome these inhibitors: coordination network, combine multiple models
- Possible solutions: liaison roles and maturity model; shared platform and new collaboration framework; better and longer (3-5 years) collaboration and reduced skills gap; building trust and continuous engagement in university-industry relationship
- The role of translator is important to translate academic research into practical solutions for companies
- They have developed a training for translator’s course (4 YouTube videos)
- Maturity model developed by Biovia is based on people, process, tools and data. Initially, investment on modelling seems reducing productivity, then the benefits come out and productivity increases (the so called “J” curve)
- Translators and Maturity Model are the two keys to overcome the current issues of academy-industry collaboration on materials modelling

Sophie Snook - ANSYS (France)

Democratization of Modelling, Simulation and Information

- Development has gone from local and linear (centuries) to exponential and global (today)
- Exponential increase of computational power (in 2023 a 1000$ computer will achieve the computing capabilities of a human brain; in 2050 of all human brains worldwide)
- Once a technology becomes digitalized, it grows exponentially (e.g. unicorn companies is increasing faster in the last years)
- Modelling can help to go from linear to exponential growth
- To do so, modelling should be democratized, reducing the enter barriers: ANSYS mission for ideation, design, manufacturing, operations and in product
- Today, simulations are used just by a few specialists and do not influence much product development. ANSYS wants to achieve 10x engineers and introduce simulations earlier in the design of products
- Currently, design engineers have to wait weeks/months to receive an opinion from technical specialists (who run simulations), and this is a bottleneck in the development of innovations. ANSYS discovery allows designers to run their own preliminary simulations; then, ANSYS flagship will be used by experts just for validation and optimization (but on a fewer amount of new ideas, thus speeding up the innovation time)
- Demo on a mechanical part of a tractor: easy to run structural FEM simulations in seconds, thus allowing an interactive change of geometrical and material modification of the design
- Demo on the fluid flow in a pipe: CFD simulations are run interactively, in seconds (just a laptop is required)
- Demo on a heat sink: FEM on temperature distribution by changing the size of pins
- Four factors are required for product development: shape (CAD), function (CAE), manufacturing (CAM) and materials (materials modelling)
- Design “the” material (lower scales) vs. design “with” material (continuum), with opposite directions between requirements and information flows
- Also, here, materials information democratization is required: creation of corporate materials information (dataset)
- Example: what if a material supplier is missing and you want to substitute with a material with similar properties? Use the corporate material database, which compare the datasheets and proposes a solution
- CES selector to identify the best material for a certain performance request

Malgorzata Celuch - QWED (Poland)

Why set up a modelling SME when you are student? The economic impact of QuickWave software

- MMAMA project by EU-H2020
- Electromagnetic modelling for microwave technology: solving Maxwell equations with boundary and initial conditions subject to material constitutive relations (continuum models)
- Applications in the communications and biomedical field
- Modelling microwaves: until 1980 heuristic, lumped, 1d models; in 1980-1990 2d and 3d models (FEM) and commercial software. Questions of engineers in 1990: will EM software help my work? Questions of engineers today: can I trust the current software?
- QuickWave software was commercialized after multiple article rejections: market is fair, if your idea is good; the business was born out of obstacles
- Why setting a business: profit, satisfaction of proof your ideas and being independent? However, the penalty are the losses and the responsibility of providing always a good product and to support your customers and employee
- Customers must need and trust your product; customer needs must be rapidly implemented; customers often prefer a fast and easy solution rather than a too accurate one
- 13 employees, 3M revenues in 2018
- Successful user stories: using QuickWave for antenna designers and producers
- Successful user stories: electromagnetic consulting & design
- EM analysis requires material parameters, which are taken from a private database (e.g. temperature dependent properties). Automatically carrying material parameters in coupled processes
- Accurate modeling of coupled electromagnetic-thermal phenomena (e.g. de-freezing of food in a microwave oven)

2.4.2 Results of the polls and related discussion

The first question was about ranking some proposed topics with regards to their economic value at industrial level (in R&D dept) vs effort (in terms of cost/resources). The results, sorted by economic value, were:

<table>
<thead>
<tr>
<th>Choices</th>
<th>effort (cost/resources)</th>
<th>economic value</th>
</tr>
</thead>
<tbody>
<tr>
<td>modellers (human capital)</td>
<td>7.92</td>
<td>8.26</td>
</tr>
<tr>
<td>physics-based modelling software</td>
<td>5.79</td>
<td>6.55</td>
</tr>
<tr>
<td>software for (big) data analytics</td>
<td>5.51</td>
<td>5.89</td>
</tr>
<tr>
<td>hardware</td>
<td>5.18</td>
<td>5.87</td>
</tr>
<tr>
<td>software platform (interoperability)</td>
<td>6.32</td>
<td>5.86</td>
</tr>
</tbody>
</table>
The emerging trend indicates that the modelers (human capital) are the most important resource in an industrial R&D department, while they are also considered costly in terms of investment. Software is considered highly impactful, with lower cost in terms of investment. According to this poll, investment on software platform (interoperability) is considered more costly than beneficial.

With regards to the collaboration between private sector and academia, the next question was: About inhibitors of the collaboration between industry and academy, how important you consider the proposed choices. The results were:

<table>
<thead>
<tr>
<th>Choices</th>
<th>Weighted average</th>
</tr>
</thead>
<tbody>
<tr>
<td>different scopes</td>
<td>3.8</td>
</tr>
<tr>
<td>different time frames</td>
<td>3.6</td>
</tr>
<tr>
<td>different language (communication gap)</td>
<td>3.0</td>
</tr>
<tr>
<td>different expertise (technical gap)</td>
<td>2.9</td>
</tr>
</tbody>
</table>
Different scopes (to generate profits vs educational and pure research projects) and time frames (project duration and different funding schemes) are seen as the most relevant inhibitors. Technical gap and different expertise are not considered critical while still above the average (2.5 points out of 5). Language gap is considered above the average threshold, while less critical than scopes and time frames.

Next question is focused on Small and Medium Enterprises (SMEs): How can SMEs best engage in materials modelling? Among the provided choices, the results were (sorted by importance):

- become partner of a consortium
- hire external consultants
- hire in-house expertise
- business decision support systems

Particular important for SMEs is considered to be the possibility to become part of a consortium. This concept has already emerged in previous meetings of the EMMC, as a good opportunity for SMEs to remedy the reduced availability in terms of budget and resources to be dedicated to R&D. Hiring external consultants – e.g. external Translators – emerges as a good choice for SMEs, while the possibility to hire internal staff and BDSS are indicated to be less critical to engage in MM.

Finally, the last question was about the degree of software code accessibility at industrial and academic level. The question was: How much share of MM software code should be accessible to industrial end users? The results were:
Industrial end users: accessible code 57%, black-box 43%
Academic researchers: accessible code 84%, black-box 16%

In general, code accessibility emerges as an important aspect to allow customization and trustiness of the obtained numerical solution, being this tendency remarkably stronger for academic users.

2.5 Session 4: Translation & Training for companies

This session was organized in the framework of the activities of EMMC-CSA Working Group "Translation and Training for Companies", and chaired by Pietro Asinari (Politecnico di Torino, Italy). The minutes of the invited talks (see also the abstract of the talks included in the program in the appendix), related discussions and instant polls for this session are reported below.

2.5.1 Report of the talks and related discussion

Peter Klein - Fraunhofer (Germany)
Translation and Training from a SMEs perspective

- Peter Klein is member of FORCE project
- Challenges in SMEs: they operate in B2B, technological specifications from business partners are clear, important time2solution and time2delivery, production volume and cost, regulations
- Typical R&D process in SMEs: customer specifies wish list, then quantify these desiderata, then discuss with customer until an agreement is achieved, then start internal R&D, constant feedback before and during the R&D. How to transform this to a modelling workflow?
- Translation begins at the R&D level, not before. Translators should highlight in which steps modelling can really be an added value
- Initial translation is typically done by external translators; after, by internal translators. They should support the complexity reduction in the model to be simulated, translating the results in the “language” of SMEs. Then, translators should also train the workforce to use and interpret the modelling results. More broadly, translators should train future workforce in academic course, e.g. summer schools
- EMMC guidelines for translators should cope with SMEs needs. The most important aspect is the constant feedback from customers
- Proposal for translators for SMEs: employ an agile approach, where early and fast feedback loops are employed. Also, costs should be taken into account as early as possible. Best approach: multi-material/criteria optimization by NASA 2040
- Best approach envisioned: kick-off meeting defining what is feasible and what is optimal, using modelling in between and trying to optimize the degrees of freedom that could be changed
- Translators request on supporting tools: models, software, hardware. Ontologies are also needed, but for domain-specific applications.
- In SMEs, training should be on the job for the internal translators, using the tools developed by external translators. E.g. training on how to use the agile methodology
- External translators should be trained at the university level, e.g. by means of summer schools. Basic economic skills are required, as well as communication skills. Of course, also a broad overview of as many modelling approaches as possible. Learning by doing working with an experienced translator
- Example: therapeutic virus production

**Fedor Goumans - Software for Chemistry & Materials (Netherlands)**

*Making new material modeling techniques technology ready & pragmatic*

- ADF was the first DFT code for inorganic chemistry in 1970s
- SCM spinoff company in 1995 to keep supporting the industrial users
- Today there are 20 employees, many academic collaborators
- 2 hired support scientist provides the translation to customers
- Case study 2: charge mobility. Paper on modelling in 2003, additional academic research in 2007, Samsung has then filed several patents
- Case study 3: sputtering deposition. In 2018 a company asked if this process can be modelled. By internal consultation, they have figured out that ReaxFF can do that, after some re-parametrization. So, in-house training can start
- SCM participate in the ReaxPro project (EU-H2020), which aims at a multiscale approach to reactive processes (e.g. catalytic reactors, from electronic to continuum models). Industrial partners are BASF, JM, DowDuPont, Shell. ReaxPro wants to overcome the valley of death between academic and exploitable codes in the field of reactive processes. The software that will be scaled-up by the project are ADF, EON, Zacros, Catalytic FOAM, which will be integrated with each other to achieve a multi-scale platform
- In conclusion: fundamental software development is useful, but translators should recognize its potential and it may take long time before economical exploitation; application-driven software development is useful, but it can be risky if too specific, duplicate of other works, help non-experts with modelling; consultancy, onboarding and active support helps adaptation, it’s all about communicating and translating
Andre Haufe - DYNAmore GmbH (Germany)

On identification of industrial needs, providing of solutions and training of clients in macroscopic constitutive modelling in engineering applications

- 120 employee, main software is the multi-physics software LS-DYNA for crash test, drop test, occupant safety, earthquake engineering and green energy
- How to identify industrial needs for crash tests. Constitutive modeling and proper meshing is the key for a reliable model. Different aspects should be coupled: damage, anisotropy, failure, plasticity, debonding, fracture growth. The goal is a predictive simulation, to avoid too many experimental tests
- Translators identify industrial needs and guide the software development. Steps: identification, implementation, verification, calibration, validation, final release
- Example 1: structures made by plastics. The mechanical response of different materials has been included in LS-DYNA after the requirement from the client
- Example 2: structures made by composites (fibers). Again, the mechanical properties of the composites (e.g. with different fiber orientation) have been included in the LS-DYNA code after expensive verification & validation. The most expensive part was the calibration of the parameters
- Example 3: damage and fraction model. GISSMO model, from forming to crash test of the component.
- Example 4: high speed impact on endless fiber reinforced polymers. H2020 Extreme project
- Conclusion: predictability and cost for calibration and execution speed are the key; Talk to the right people: OEM pave the road, SME will follow; Set up a diverse team that loves the job; Do not hide problems during verification and validation; Dissemination: talk about the novelty in conferences, papers, seminars, lectures, ...

Svenn Halvorsen - NORCE (Norway)

Model Translator – What Is Required?

- The modelling process: preparation, modelling work, validation and post results processing
- Translator needs to know the audience
- Use non-dimensional equations to simplify their description to a non-technical audience
- Required accuracy for the mathematical model changes according to the application field (+/- 10% vs +/- 1%)
- “All models are wrong, but some are useful”
- A translator should have strong business/technical skills and also communication skills (active listening, questioning techniques, presentation skills). He/she has to understand what is needed and what is wanted, what is observed (not questionable) and what is the interpretation (questionable), has to keep integrity, know his/her limitations and where find help,
- BALA sales model: Need, Acceptance, Solution, Acceptance
- Gap to mathematics is due to the personality type of each one: the translator should be able to understand the value of each personality type and modulate the language according to it

2.5.2 Results of the polls and related discussion

The first question posed to the audience was related to the skills that Translators should have and their importance in the overall expertise: How important are for translators? And three options were ranked as follows:
Soft skills - 4.1 out of 5  
Modelling skills – 3.9 out of 5  
Business concepts – 3.5 out of 5

It turns out that soft skills are considered to be critical for Translators – concept that had already emerged during previous meetings. Technical skills are then considered more important than economic concepts – demonstrating the requirement of having solid technical background for Translators, yet economic concepts are anyway above the average threshold of 2.5.

Next question was devoted to have insight on the market and room for employment of Translators. So, the question was: In your opinion, how is the market divided between and three given options were ranked as follows:
In raw form:

Process consultants – 47%
Materials consultants – 30%
Materials modelling consultants – 22%

According to the audience of this meeting, most of the market of materials is available to process consultants, secondly to materials consultants and ultimately to MM consultants (Translators). This result is in line with other considerations on the still moderated uptake and use of MM techniques at the industrial level.

Focusing on training for Translators, the next was question was oriented to understand at which level should a specific career/course/cycle be planned for the specific Training of Translators. So, the question was: Regarding training of translators: at which level should a specific training course be planned?

The audience ranked first the PhD course level, yet almost equally to the post-doctoral level. Master level results to be less appropriate for this case. This result is in line with the very solid technical background that a Translator should have, which can be achieved during master level courses. The expertise can then be complemented with ancillary concepts oriented to technological innovation for industry at PhD and post-doc level – i.e. economic concepts and soft skills. In general, the trend shows that solid preparation is required for refinement of the skills.

Finally, the last question was focused on the (near) future of Translators: Your keywords for Translators in the next 3-5 years (open response). The resulting word cloud is shown below, being the bigger words those occurring more frequently in the responses. Most frequently indicated words indicate that digitalization, machine learning and workflow will be key to Translators in the very next future, in line with migration to (big) data and IoT (Industry 4.0).
2.6 Session 5: Interoperability and integration

This session was organized in the framework of the activities of EMMC-CSA Working Group "Interoperability and Integration", and chaired by Gerhard Goldbeck (Goldbeck Consulting, UK). Particularly, this session was included in the meeting as the “Open Simulation Platforms, Interoperability for industrial application” (Expert Group Meeting organized by the same group). The minutes of the invited talks (see also the abstract of the talks included in the program in the appendix), related discussions and instant polls for this session are reported below.

2.6.1 Report of the talks and related discussion

Gerhard Goldbeck & Jesper Friis - Goldbeck Consulting (UK) & SINTEF (Norway)

EMMO: A semantic knowledge framework for materials and modelling

G. Goldbeck gave an overview of the EMMO and J. Friis tackled application issues and showed how one can use the EMMO. The demo example was modelling the Mechanical response of welding Al onto a steel plate. Therefore, it is necessary to couple tool starting from DFT (electronic) to continuum models. The EMMO is needed that interoperability between these tools and granularities can be accomplished.

Across different scales, we can identify the following components for example: at the macroscale, we have the complete welded structure between a layer of Aluminium and another one of Steel. At the microstructural level, we have the intermetallic phases and interfaces, for example composed of alpha AlFeSi, theta Fe4Al13 and nu-Fe2Al5. Finally, at the atomistic/electronic level, we have the atomistic crystal and interface structures. To different length scales also correspond different transferred properties: for example, from atomistic structure one can compute the interface traction separation and the bulk elastic constants, which are then transferred into the microstructure level through which the cohesive behaviour of the structural elements can be computed, and so on until a complete understanding of the mechanical response properties of the overall welded structure is obtained.

As OWL itself is not suitable for complex scientific data, J. Friis and co-workers have developed emmo-python – a Python API for the European Materials & Modelling Ontology (EMMO) which can be found here:
https://github.com/emmo-repo/EMMO-python. Emmo-python is based on Owlready2 and provides an intuitive representation of EMMO in Python.

Note: Owlready2 is a module for ontology-oriented programming in Python 3.

The ontology is used to map input and output properties which is needed as first step to enable interoperability.

User cases can also be represented as MODA workflows. For example, at the level of atomic structure, the model consists in electronic structure/DFT, as represented by the Kohn-Sham Equations, then the raw output consists in the self-consistent energies, and finally the processed output in physical quantities such as the traction separation and the elastic constants. Such processed output can then be fed into the workflow representing the microstructure geometry at the continuum level, where this time the theoretical model is embodied by Newton’s 2nd Law resulting in the calculation of the mechanical forces (stress tensor), and finally in the generation of processed output such as the cohesive response of the aluminium-steel welded interface and, at an even higher continuum level, the failure conditions of the welded components.

From the perspective of an ontological representation of the user case, the DFT input properties such as atomic positions, lattice vectors, atomic masses and atomic numbers are related to the corresponding DFT output properties via the various types of relations. Examples of output properties include traction separation and stiffness tensor.

Note: the stiffness tensor is a property of both the crystal unit cell (atomic level) and of the representative elementary volume (continuum level). This demonstrates an example of vertical interoperability. Physical quantities such as stiffness tensor, atomic number, lattice vectors etc… can each be represented as a distinct class in the python representation of the ontology. In order to realize the interoperability between applications via a common ontology, we have to provide a mapping function between these applications and the common ontology.

The approach we consider is to use a metadata framework: generate metadata from common ontology, define application metadata, instantiate application data, and finally map the application data to an instance of the common metadata.
A C implementation of the SINTEF Open Framework and Tools (SOFT), which is free and open source (MIT license, located at https://github.com/jesper-friis/dlite) is used to get a meta data centric framework by generating metadata from the EMMO.

Metadata schema look like:

<table>
<thead>
<tr>
<th>Name</th>
<th>Type</th>
<th>Dims</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>e-bonded_atom</td>
<td>metadata</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>UUID</td>
<td></td>
<td></td>
<td></td>
<td>87134b67-9a0b-5a80-8380-74b3e74a2c2b</td>
</tr>
<tr>
<td>URI</td>
<td></td>
<td></td>
<td></td>
<td><a href="http://emmc.info/emmc/demo/0.1/e_bonded_atom">http://emmc.info/emmc/demo/0.1/e_bonded_atom</a></td>
</tr>
<tr>
<td>Meta</td>
<td></td>
<td></td>
<td></td>
<td><a href="http://meta.sintef.no/0.3/EntitySchema">http://meta.sintef.no/0.3/EntitySchema</a></td>
</tr>
<tr>
<td>Description</td>
<td></td>
<td></td>
<td></td>
<td>An electronic bonded atom that shares at least one electron to the atom-based entity of which is part of.</td>
</tr>
</tbody>
</table>

Piotr Maciol - AGH University of Science and Technology (Poland)

The prototype ontology for metal alloys

P. Maciol is interested in modelling the heat treatment of metal alloys and as this is a very complex phenomena, which requires multiscale modelling. In this spirit, several years ago the speaker’s university department started developing agile and adaptive multiscale modelling methodology (AM3), to provide a framework for adaptive multiscale modelling. To make these models interoperable an ontology is needed as knowledge-based rules are turned out to be not sufficient enough.

The core items of the phenomena under investigation are precipitation and phase, the core classes are phase, origin, location, and shape. The models needed to be linked are macroscale and mesoscale.

Precipitation kinetics is one of the phenomena occurring during heat treatment of metal alloys. It leads to particles nucleation and growth in solid solutions (metal alloys). Precipitations sizes, number and locations influences mechanical properties of metal alloys, and leads to precipitation hardening. From an ontological perspective, this phenomenon can be described by the core items, such as precipitation and grain, and core classes, such as precipitation type (phase, origin, location, shape) and Matrix phase. Precipitation kinetics is also a multiscale model, which can be described at the macroscale (Heat transfer, Plastic deformation and Yield stress), and Mesoscale (number, shape, location and type of precipitations, as well as the main phases grains, described by their shapes, fraction, and morphology). The linking properties between the two length scales can be defined in both directions, either by downscaling (temperature, deformation rate), or by upscaling (mechanical properties...
such as yield stress, dependency on grains and precipitations morphology). The model is designed for a specified alloy (or narrow family).

P. Maciol looked into the EMMO and the RoMM and took the PE&MR concept and the granularity. Working with the EMMO requires knowledge of OWL2 and Protégé which could be acquired. Also, a taxonomy for aluminum alloys had to be developed. To do all of that correctly an expert consultation would be required and some curation once a new branch needs to be added to the EMMO. Provision of examples would be highly appreciated and more tools.

In summary the EMMO is seen as helpful but very complex.

**Ian Bruno - Cambridge Crystallographic Data Centre (UK)**

*Achieving Interoperability between Crystallography and Chemistry*

The Cambridge Crystallographic Data Centre is an International Data Repository providing an archive of crystal structure data. It is a Collaborative Research Organization, where New methodologies are developed, and Fundamental research is carried out. It is also a Scientific Software Provider, where search, analysis and visualization tools as well as scientific applications are developed. It is furthermore involved in education and outreach, via conferences, Workshops, Training, Teaching.

It originated in 1965 as a non-for-profit UK Registered Charity and University Partner Institute. CCDC is today dedicated to the advancement of chemistry and crystallography for the public benefit through high quality information services and software. Some statistics about CCDC: over 1 Million small-molecule crystal structures, over 80,000 datasets deposited annually, links to over 1,000 journals. It is enriched and annotated by experts, and the structures are available for anyone to download.

The aggregation of experimental datasets provides a foundation for resources that enable structural knowledge to be applied to scientific challenges across sectors and domains. Association of chemistry and crystallography is in fact key for enabling discovery of new insights. This effort manifested in a number of recent papers, where people have been using the CCDC platform to look at a range of different applications involving data, for example to estimate melting temperatures, looking at organic electronics’ energetic materials, or whether or not these substances will crystallize. A lot of these studies were based on machine learning techniques.

However, if these Machine Learning applications are to be successful, you really do need to make sure that you have good quality data underpinning. If your data is bad, machine learning tools are useless. You therefore need good quality data to begin with.

Machine learning requires many and well curated data; thus, the FAIR data principle is key. This means that data should be findable, interoperable, accessible and reusable both by humans and machines.

The crystallography community uses CIF files which are semantic representations of crystal structures. CIF is quite useful and supports exchange protocols, based on data dictionaries and relational rules. Using a tool called “checkcif” can validate data before they are submitted into a repository. This tool checks consistency and integrity of the data and generates alerts that should either be corrected or explained. Its report and explanations can be embedded in the CIF file directly.

The IUPAC International Chemical Identifier (INCHI) is introduced as standard chemical identifier (https://iupac.org/who-we-are/divisions/division-details/inchi/), that can be used in repositories such as ORCID. The IUPAC goldbook (https://goldbook.iupac.org/) was introduced as compendium of chemical terminology. Also, other communities were thriving towards unified file formats such as the spectroscopists with JCAMP and the Allotrope Foundation around analytical machinery. A recent (2018) EU report (https://www.ouvrirlascience.fr/wp-content/uploads/2019/03/Cost-Benefit-analysis-for-FAIR-research-data_KI0219023ENN_en.pdf) states the not having FAIR data costs the European Economy € 10.2 bn/annum. Digitizing and digitalization will bring changes but only if the data are FAIR. The main goal is to use this data for machine learning, so semantics and ontologies will have to play a role.

Concluding thoughts:

- Applying the FAIR data principles to your data potentially releases significant value and increases efficiency
- Interoperability of data is greatly aided by standard formats, identifiers and vocabularies
- Development, adoption and maintenance of effective standards requires input from stakeholders across the board

2.6.2 Results of the polls and related discussion

The first question of this session was preliminary devoted to highlight the expectations about ontologies. So, multiple options were provided to the question: What is the main expectation about ontologies? And the audience ranked the provided options as follows:

1. improved interoperability and exchange
2. better integration across domains
3. more effective analysis
4. better data documentation
5. easier querying
6. improved decision making
As expected, easier exchange of data ranked first, with better integration across domains being also a very relevant expectation. Improved decision making ranked last, probably due to being actually a hidden consequence of a better interoperability.

Audience was then asked to provide ideas to lower the barrier to the adoption of new ontologies. The results are reported in the figures below.

And in raw form:

- workshops
- Training by simple examples, well documented
- Hands-on examples
• Good examples
• Show us how to practically make use of it/them
• Training
• A lot of well documented cases
• Tools
• Training
• Better more intuitive documentation
• User examples and tooling
• Effective case studies
• Organized simple documentation
• Case studies and examples
• Tools and examples
• Training, Demonstration case studies
• Use more intuitive terminology
• Optimized APIs and docs
• Make ontologies intuitive
• Clear and general framework
• Examples, practical workshops
• Organizing Workshops, webinars
• Give practical examples
• Sharing knowledge between stakeholders
• Show advantages through examples and case studies
• Take into account community language/needs when developing them
• examples
• training, workshops, common ontologies for materials processing
• provide services from the national and international institutes: European Commission, NIST, National institutes of standards
• Tools optimized
• more friendly

A clear emphasis on (successful) application cases and examples emerges from the responses of the audience. This may be eventually associated with relatively low knowledge of the potential of these tools for interoperability, which requires better documentation.

Finally, the last question was about the development of new ontologies: Who should develop ontologies? Provided options ranked as follows: academic IT scientists, Translators, software providers and analytical philosophers. Actually, the trend indicates that IT scientist should be more involved into the development of the ontologies, being also Translators considered important in this process. Analytical philosophers ranked last, from the responses of this audience.
2.7  Session 6: Artificial intelligence & Industry 4.0

This was an additional special session, organized to be complementary to the EMMC-CSA activities, and chaired by Eliodoro Chiavazzo (Politecnico di Torino, Italy). The minutes of the invited talks (see also the abstract of the talks included in the program in the appendix), related discussions and instant polls for this session are reported below.

2.7.1  Report of the talks and related discussion

Salvador Izquierdo - ITAINNOVA (Spain)

Translation of physically-informed data-driven models of material transformation processes

S. Izquierdo introduces ITAINNOVA, https://www.itainnova.es/es. It is a research technology center located in Zaragoza (Spain), mainly oriented to materials modeling, characterization and processing. S. Izquierdo is leading the Multiphysics & Multiscale Simulation Group. The speaker presents some example of technological challenges related to projects his group has been involved into. This leads the speaker to state that a systematic approach is needed to better control and optimize materials processing – given that uncertainties can hinder the quality of the final product if not properly taken under control. In the context of industrial digitization and Industry 4.0, this systematic approach is proposed in the form of CAELIA (https://github.com/caeliaITAINNOVA), a library for building smart applications for workflows in materials processing. CAELIA is described as a modular framework to build “Digital Twins” of specific systems. CAELIA is based on modules with different purposes, which allows acquisition of data where needed (IoT) which are used to develop a reduced model within an incremental loop. The model is built using tensor factorization for unstructured data and is refined until the desired degree of representation/fidelity of the physics of the problem. Additional data is inserted into the model developer until satisfactory results are achieved. The speaker states that in this view, accuracy can be basically controlled. The potential of the proposed platform is discussed in terms of simplification of the user’s actions and automatization of the model building process. A perspective view on possible use from different community is given.
Haoyan Huo - University of California Berkeley (US)

Data-mining millions of scientific literature for predictive materials synthesis

H. Huo introduces himself as being PhD student in the group of Prof. Ceder at the University of California at Berkeley and Lawrence Berkeley Lab - [https://ceder.berkeley.edu/](https://ceder.berkeley.edu/). This group is very big (around 30 people among PhD students and post-docs) and is focused on materials modelling all round with particular emphasis on physical-chemical properties. Besides, and along with this axis, the group is keen to explore ML solutions and data analysis. In this talk in particular, the main topic is materials synthesis. Indeed, along with exploration and eventual discovery of new materials via modelling and simulations, synthesis often represents a bottleneck, as some newly screened materials are very difficult to synthesize and therefore their practical production is very difficult and requires year of trial and error experiments or even not possible – i.e. correct synthesis is not found. An extensive source of synthesis procedures can be found in technical literature. Extracting and systematically organizing materials and related synthesis techniques greatly helps in finding solution for and insights for newly proposed materials. They have thus set-up a machinery for automatic literature screening and mining, to extract relevant procedure for the synthesis. The literature data set consists of several millions of papers, from which sentences related to synthesis procedures have been analyzed using Natural Language Processing and Machine Learning. A data set around 20k synthesis reactions has in this way been obtained.

Rajat Srivastava - Politecnico di Torino (Italy)

Thermal properties of nanomaterials predicted through atomistic-to-continuum models supported by machine learning

R. Srivastava works at the Multi-Scale Modelling Laboratory ([www.polito.it/small](http://www.polito.it/small)), Department of Energy at Politecnico di Torino as post-doctoral researcher. The talk is about thermal properties of nano-composites (epoxy matrix + carbon nanofillers). This activity relates to H2020 project namely MODCOMP, [http://modcomp-project.eu/](http://modcomp-project.eu/). Interest is in the computation of thermal conductivity of the composite materials for several different industrial applications, from automotive to biomedical. A multi-scale technique is adopted to obtain the effective thermal conductivity of epoxy matrix + carbon nanotubes. All-atom simulations are carried out to compute thermal and interfacial properties for filler-filler and filler-matrix systems. Thermal conductivity and Kapitza resistance are computed for different e.g. filler orientation and several other parameters in a sensitivity analysis. Next, these obtained properties are used in a mesoscopic model to compute the effective thermal conductivity of carbon-reinforced composites supported by ML tools. Several FEM simulations are performed to compute the shape factor between carbon nanotubes at different scenarios (20k simulations). The results are best-fitted using ML tools and incorporated in the mesoscopic model to compute the thermal conductivity of the composite and verified with experimental data.

2.7.2 Results of the polls and related discussion

The first question was about the general trust of the users between physics-based and data-driven modelling results: Assume that you have enough (training) experimental data, what would you trust more on the same phenomenon? The results is reported below
Actually, the audience ranked 67% of trust in physics-based models, demonstrating still a certain lack of confidence in data-driven modelling (early technology).

The next question was about the hidden cost of AI/ML. That is, a comparison between the time spent for the development of the algorithm with respect to the potentially saved time in R&D projects. In general, the audience indicated that the effort is worth, the perspective time saved using automatic AI tools ranked 55% in terms of potential time saved with respect to the time that invested for the development of the machinery (45%). This latter percentage is quite high and may be associated with the still early maturity of these technologies and their still relatively low widespread adoption in industry.

Next question was about the role of Translators in the digitization of the EU industry: How will Translators help in digitization of the EU industry? This was left as an open question and audience was asked to provide ideas. The results are reported below:
And in raw format:

- Assembling test cases
- Training, development of tools, software
- Uptake of molecular/mesoscopic modelling by industrial engineering practice
- Systematizing the company data and making the expectations more realistic
- Depends how good the translators are
- Bridge a Communication gap
- Developing AI-MM workflows
- They should find reasonable way and domain to be digitized
- Develop ontologies and data acquisition templates
- Providing answers to on-going issues with new tools
- Setting the rules to develop tools
- Development successful solutions for customers using available modelling tools, training, support right ontologies
- Combining machine learning and physical models
- Introducing new technologies to the industry
- Connect experts and business decision makers
- Opening new markets

The trend from the given responses seems to be oriented to dedicate Translators to ease the process of uptake of data-driven tools in industry and development/adoption of new ontologies for data interoperability. This aspect may be taken into account, in perspective, on the role of Translators and their training.

Finally, the last question was about training of data-driven modelling and mining: What should be the background to teach courses on AI for MM industrial needs? Responses are as follows:
According to the audience, modelers (9 choices) and mathematicians (7 choices) should be involved into training of these topics in a priority manner. Computer scientists (5 choices) and IT (1 choice), which are actually very similar with the former being more oriented to implementation of modelling tools and the latter to communication and data exchange. From the raw responses, even summing up Computer scientists and IT scientists, this block remains at the last place, with modelers and mathematicians being the most proper to train these topics in any case.

2.8 Poster Session

The posted session, held on Tuesday July 9 in the afternoon, included 14 poster that were exposed during the whole meeting for discussion and interaction:

1. Cinzia Giannini - X-ray Microlmaging Laboratory (XMI-L@b)
2. Cinzia Giannini - SUNBIM: a package for X-ray imaging of nanomaterials and biomaterials using SAXS, WAXS, GISAXS and GIWAXS techniques
3. Javier Gomez - A machine learning application to mechanical and fracture material characterization
4. Martin Thomas Horsch - Molecular model database of the Boltzmann-Zuse Society for Computational Molecular Engineering
5. Amaya Igartua - Modelling activities as a tool to optimize materials, products, process and performance
6. Otello Maria Roscioni - A Reversible Coarse Graining Model for Organic Functional Materials
7. Fabio Sacconi - TiberCAD: a tool for multiscale simulation of nanostructured devices
8. Massimo Celino - EoCoE: the European Energy oriented Centre of Excellence
9. Lorenzo Chiavarini - iMat: Data extraction from scientific papers through Machine Learning
10. Paolo De Angelis - Exploring the free energy landscapes to predict surfactant adsorption isotherms at solid-liquid nanoscale interface
11. Silvia Chiacchiera - Explicitly polarisable mesoscale (DPD) models for water
12. Malgorzata Celuch - QuickWave conformal FDTD modelling: electromagnetics and beyond
13. Gabriele Falciani - Multi-scale modelling of transport phenomena through engineered soap films for fuel generation
14. Xavier Alvarez - Multiscale model for thermal transport at the nanoscale: From ab-initio to Finite Elements description
A mini-presentation session (1 min per person) was organized to enhance and promote the visibility of the presented posters (abstracts are available in the program of the workshop in the appendix of this document). A mini session poll was organized on Wednesday 10, to choose the best poster presentation).

Poster number 9, according to the audience resulted to be the winner.

3. Conclusions

This meeting was planned to encompass the EMMC activities all round and represented the last extended workshop in this sense before the end of the EMMC-CSA project in August 2019. The event gave the possibility to discuss activities on: Model Development and Validation, Interoperability and Integration (expert meeting on Open Simulation Platforms, Interoperability for industrial application), Translation and Training for Companies, Industrial Software Deployment (expert meeting on cloud-based solutions), Industrial Integration and Economic Impact (expert meeting on Tactics for enterprises). Besides targeted invitations of the invited speakers per session, the EMMC community has been informed via the EMMC contact list and invited to participate. Remarkable interest has been received to attend from the community, demonstrating the success of the previously organized meetings and the credibility of the EMMC events as an occasion for fruitful discussions for the materials modelling community. The participation was well distributed among industry, academy and Research Technology Offices. According to the feedback received from the attendees after the meeting, this event has been very appreciated in terms of quality of proposed contributions (talks and posters) and discussions promoted by the interactive polls, organized to promote inclusive participation and collection of feedback. The specific conclusions obtained from the digested feedback per session are reported next.

Session 1: Materials modelling techniques

The first talk was from Elisa Molinari (CNR, Italy) about the Max center of excellence. MaX is one of the EU centers of Excellence for HPC applications, supported by the EU under the H2020-INFREADI-2018-1 project. The center supports the developers and end users of advanced applications for materials analysis, at the frontiers of High-Performance Computing (HPC) and High-Throughput Computing (HTC). It works to towards enabling the exascale transition in the materials field, by advanced programming, novel algorithms, specific libraries, data management, software/hardware design and technology-transfer. It offers: consulting, training and support. Second talk was from Arnulf Latz of the German Aerospace Center (Germany). The talk was about modelling batteries, with particular emphasis on multiscale modelling (from electronic to continuum). Application is mainly related to degradation. The third talk was from Vladimir Lobaskin of the University College Dublin (Ireland) about modelling of bio-nano interfaces (interfaces/interaction between organic and inorganic materials). Applications involve, among others: therapy, drug delivery and nanoparticle toxicity. Challenges in the filed include: lack of force filed, lack of information, different time scales. Both physical understanding and
experimental data driven modelling are very important in the field. Finally, the last talk was from Ilian Todorov of the Science and Technology Facilities Council (UK). The talk was about the DL_MESO code, which is a general-purpose mesoscale simulation package developed in Fortran 2003 and C++ and supports Lattice Boltzmann Equation (LBE) and Dissipative Particle Dynamics (DPD) methods. It is supplied with Graphical User Interface (GUI) and is capable of both serial and parallel execution. DL_MESO is free for academic scientists (non-commercial use) and license can be acquired by commercial organizations.

The first discussion topic for the polls was about the requirements of the industrial sector from a material modelling point of view. The audience indicated that, ready-to-go solutions for identified challenges and better evidence that MM can be an added value are critical aspects in this sense. With regards to model types, at the industrial level, it turns out that continuum models are still considered very impactful (due to the high maturity level), while electronic models are considered less potentially impactful (in general). Coupling & Linking of models is considered important from an industrial perspective, yet it is considered costly in terms of expertise for development and adoption. Finally, the last question was about how to increase industry's trust in materials modelling. The audience ranked the following options in this order: Benchmarks for verification & validation of models, More accurate materials models and techniques, Advance uncertainty quantification (UQ) methods. This actually gives particular importance to V&V as a critical aspect to consider towards better uptake of materials modelling in industry.

Session 2: Software deployment

Within the general focus of WP5 on the stimulation of industrial deployment of materials modelling software this session, which was also organized as an expert group meeting on “Cloud-based solutions”, centered about the chances and risks of web-based platforms aiming at more efficient ways to bring together all stakeholders. In particular, the idea of such platforms is to enable industrial end users to quickly identify partners and software helping to solve the problems these researchers are faced with. In return, software developers and consultants would be able to make their solutions and expertise readily available to a broader community of industrial researchers.

The first speaker was Beatrice Carasi from COMSOL (Italy), who discussed first trends in what industry needs, that can be recognized mainly in thermal management and production / harvesting of energies and, in perspective, additive manufacturing, digital twin concept and internet of things (IoT). The success of COMSOL particularly relies on: (i) support, (ii) integration and (iii) robustness. The most important aspect is to listen to the users’ need and feedback. Second speaker was Umberto Martinez - Synopsys (Denmark). He spoke about the development of QuantumATK platform using the SCRUM. The talk has been particularly focused on the methodology that the company adopts for agile code development (specific expertise, feedback, meetings and discussion of problems for ready solution and cooperation by the developer team). Gabriele Mogni from Exabyte.io (US), presented the platform being developed from the company, with some example of the use on the cloud. He discussed some of the advantages of cloud computing, such as: 1) Avoid investments in in-house HPC hardware infrastructure which becomes obsolete 2) using only a web browser, which allows access even from a smart phone, 3) the general accessibility of the cloud by all (allowed) end users of a company, which makes the cloud a highly collaborative ecosystem, 4) the flexibility of choosing service level and licensing schemes, and 5) the freedom from buying software licenses. In addition, according to the speaker, cloud computing is ideally suited for materials modelling as data transfer is usually very little.
Guided by the three keynote talks this session discussed the perspectives of platforms such as online marketplaces and cloud solutions. The speakers emphasized the importance of good communication between software developers/owners and industrial end users/researchers for optimal response to the end users' needs. This also requires lean and agile software development techniques such as SCRUM, which allow fast implementation of new features, permit regular feedback, and minimize the risk of failure. An alternative route to close developer-end user relationship is offered by cloud computing, which offers a high degree of flexibility regarding the use of computational resources. Yet, due to IP, security, and data-safety issues industry is still reluctant taking up such solutions. The crucial role of these issues was also seen by most attendees. Overall, this expert meeting/session provided a broad overview of current and future trends of the interaction between software developers, software owners, and industrial researchers. While the present audience was split into two groups of equal size regarding midterm expectations on the preference of in-house computing and cloud-based solutions the coming years will provide a clearer picture of the roles these two models play for industrial materials modelling.

**Session 3: Economic impact of materials modelling**

Several points mentioned in the presentation have been discussed. The first point is the need to move away from linear models and approaches. Exponential adoption of digitalized technology, high complexity in collaboration due to multi-stakeholder environments has been mentioned in all the talks.

Another common point is the need to increase the users and impact of materials modelling, through democratization, validate workflows, easy to use software. It has been estimated that in engineering simulation environment democratization strategy can increase the number of simulation users by an order of magnitude.

Another point of discussion was related to the gaps between academia and industry, specifically how to move proof of concept to high TRLs, required by industry adoption. While there is the consensus on the need for dedicated founding, it has been raised the question if increasing of codes' TRL has to be done by of universities or rather of software companies and/or RTOs.

The last point of discussion was the trade-off between black-box (regarding the source code) and visibility/accessibility of code. Software developers (micro to macro business) prefer to keep the code consolidated; it is difficult when end-users try to manipulate the code themselves, in addition it was pointed out that successfully modify a commercial code without specific training and guidance is not an easy task even for developers. The debate black-box vs open codes also highlighted the different requirements between academic researchers which prefer to be hands-on with the code and industry actors which may prefer to be less hands-on with the code. Within either option it was generally agreed that the implemented models should be documented at least in a form of MODAs.

**Session 4: Translation & Training for companies**

Session has been devoted to impulse presentation for discussion of the role of Translators and their training. The first talk provided by Peter Klein from Fraunhofer (Germany) was particularly focused on Translation activities for Small and Medium Enterprises (SMEs). The speaker first described the specific challenges in SMEs in R&D processes, and how translators (firstly external then internal can help). In this context, Translators may also act as trainers, which is an added value in the context of the whole Translation process. The second talk
was given by Fedor Goumans (UK), and was about promoting the access to materials modelling techniques at large. The speaker first introduced the company (SCM) and presented different case studies related to materials optimization in industrial context. This allows to show how SME such as (SCM) handle these activities. The speaker also shows how participation in EU projects is beneficial to a software SME. Third speaker was Andre Haufe from DYNAmore (Germany), who spoke of Translation in the context of industrial continuum modelling (solid mechanics) with different examples. Main addressed points were: predictability and cost for calibration and execution speed are key; need to talk to the right people: importance to set up a diverse team that loves the job; do not hide problems during verification and validation; importance of dissemination. Finally, the last talk was given by Svenn Halvorsen (Norway). He spoke about the Translation process in general, with focus on the importance to: listen and understand the problems, the Translators’ attitude and character, the Translators’ skills.

With regards to the polls, they have allowed to collect feedback on the skills required by Translators, i.e. the balance between technical, economic and soft skills. The audience indicated soft skills to be very important, confirming what already emerged in previous meetings. The polls also indicated that, according the present audience, the materials market is eminently available to (in this order): process consultants, materials consultants, and materials modeling consultants. Regarding training, thinking about the possibility to establish a tailored course for Translators, we asked the audience at which level it should be eventually planned. The audience is almost equally divided to best plan it at PhD or post-doctoral level, while a smaller part of the audience indicated Master level. Finally, thinking about the Translators’ role in the next 5 years, we have asked the audience to provide the most meaningful keywords. The most indicated were: “workflow”, “machine learning”, “artificial intelligence” and “agile”, indicated that, as expected, Translators will be involved in the digitalization of the EU industry and their training will thus need to take this issue into account.

**Session 5: Interoperability and integration**

This session has highlighted the need to develop ever more comprehensive and flexible ontologies for the sake of making multi-scale modeling techniques better integrated and inter-operable with each other. There is in fact to this day a problematic lack of conventional terminology and exchange of information on relationships between the concepts and properties involved in different materials modelling techniques, for example atomistic and continuum modelling.

The European Materials & Modelling Ontology (EMMO) has already accomplished a significant step into this direction of improved interoperability. It provides a framework to integrate materials data and models into a coherent, science-based knowledge system, enabling interoperability and enhanced decision making based on a combination of data (statistics) and reasoning (logics).

However, the relatively high abstraction level of EMMO still makes it necessary to develop customized ontologies for particular domains. This is what motivated Piotr Maciol and co-workers to conceive a new innovative ontology prototype, consistent with EMMO, dedicated to the representation of metal alloys. It was designed to support interoperability of several numerical models used in multiscale modelling of precipitation kinetics in aluminum alloys.

Another important effort in achieving an improved interoperability between Crystallography and Chemistry was accomplished by the Cambridge Crystallographic Data Centre (CCDC), via their maintenance and development of one of the most advanced and comprehensive databases of experimental organic crystallographic information
in the world. Key to the success of the CCDC was enabling interoperability of crystallographic and chemical data and activities, with the aim to enhance their adoption among the global scientific community. The criteria for interoperability in this case are based primarily on the FAIR Data Principles, which highlight the need for standard formats for knowledge representation and associated vocabularies. Within the domain of crystallography, the Crystallographic Information File (CIF) largely satisfies these requirements by enabling semantic representation of many facets of a diffraction experiment. Another aspect of interoperability is the ability to reference between data resources. Here, standard identifiers are key and the IUPAC International Chemistry Identifier (InChI) is an important enabler of links to chemical data resources.

Session 6: Artificial intelligence & Industry 4.0

This was organized as a special session, not strictly included in the original program for the meeting and has been planned to be complementary to the others in view of the ongoing digitalization of the EU industry. In particular, the objective was to have some insights and points for discussion about the perspective exploitation of Artificial Intelligence in the segment industrial innovation in the materials modelling field.

To this purpose, some eminent examples of how these tools can be adopted to benefit of modelling, yet not only, have been proposed and discussed. First, Salvador Izquierdo from ITAINNOVA (Spain) presented a novel platform under development, namely CAELIA, that combines experimental data retrieval (i.e. lending towards IoT) with reduced order-modelling techniques to automatically adjust and refine materials processing models using a “retroaction” logic. This represented a good example of integration of different techniques and data types to the benefit of materials processing control and optimization along with automatization. Second, Haoyan Huo, from the University of California Berkeley, presented a smart algorithm that have been developed to automatically extract meaningful information (mine) literature papers. The algorithm has been used to screen and extract synthesis procedures from scientific literature using Natural Language Processing techniques. This has allowed to process a very large amount of available information (millions of papers) and extract thousands of procedures for known materials synthesis in a systematic way. This result is remarkable, as synthesis often represent a bottleneck for realization of new materials, envisioned by e.g. high-throughput simulations. These techniques have, without any doubt, great potential for systematic screening and mining of literature data for other applications. Eventually, these techniques may be also complementary to modelling. Finally, Rajat Srivastava from Politecnico di Torino, presented a multi-scale modelling approach to obtain thermal properties of carbon reinforced polymeric composites using ML-based tools.

Related to the previous contributions, the proposed questions for the poll to the audience have allowed to rise the following major discussion points. 1)  simulation-based results seem to be still more trusted than those that can be obtained via AI-based predictions (from available data). However, during the discussion opinions indicate that these tools are increasingly been trusted and will to get more and more importance at the industrial level. At the moment, the effort for the development of AI tools is still considered important with respect to the final benefit in terms of later time saving. Perhaps, with the increasing maturity level of AI, this balance would be in the future more projected to the benefits with respect to the development effort. A role for Translators clearly emerged from the audience in the context of digitalization and Industry 4.0. In order to be ready for this, Translators may get ready with complementary knowledge on big data handling and (AI) mining tools. So, their training, should encompass these aspects.
4. Acknowledgments

Luca Bergamasco (POLITO) would like to sincerely acknowledge Dr. Matteo Fasano and Dr. Annalisa Cardellini (POLITO), who were attending the meeting as external experts, for contributing the raw minutes of Session 3/4 and Session 1, which have been used to shape the related parts of the present document.

5. Appendix 1: Workshop program

The final program of the workshop is submitted as an integrating attachment of this document.
**Authors**  
Luca Bergamesco, Matteo Fasano, Annalisa Cardellini (all POLITO)

**Contributing partners**  
POLITO, GCL, MDS, HGZ

**EC-Grant Agreement**  
723867

**Project acronym**  
EMMC-CSA

**Project title**  
European Materials Modelling Council - Network to capitalize on strong European position in materials modelling and to allow industry to reap the benefits

**Instrument**  
CSA

**Programme**  
HORIZON 2020

**Client**  
European Commission

**Start date of project**  
01 September 2016

**Duration**  
36 months

**Consortium**

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**Coordinator – Administrative information**

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<th>Nadja ADAMOVIC</th>
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8-10 July 2019
Sala Teatro, Links Foundation (SITI)
Corso Castelfidardo 30A, 10129 Turin
Politecnico di Torino – Turin (Italy)

Meeting organization
Pietro Asinari and Luca Bergamasco
Department of Energy - Politecnico di Torino

Web page of the meeting
https://emmc.info/events/emmc-torino2019/
PROGRAM

Monday 8 July 2019

11:45 - 12:45 Welcome lunch
11:45 - 12:45 Registration opening
12:45 - 13:00 Welcome by Prof. Roberto Zanino, Deputy Rector for European Relations
13:00 - 13:10 Welcome by the European Materials Modelling Council

Session 1: Materials model development
Chair: Kersti Hermansson (Uppsala University, Sweden)

13:10 - 13:15 Introduction and focus by session chair
13:15 - 13:45 Elisa Molinari - University of Modena and Reggio Emilia (Italy)
   Designing materials with HPC: the MaX European Centre
13:45 - 14:15 Arnulf Latz - German Aerospace Center (Germany)
   Spatially resolved modeling and simulation of degradation in Lithium ion batteries
14:15 - 14:45 Vladimir Lobaskin - University College Dublin (Ireland)
   Multiscale modelling of bionano interface
14:45 - 15:15 Ilian Todorov - Science and Technology Facilities Council (UK)
   DL_MESO: The UK’s DPD Vehicle for Academic and Industrial Collaboration
15:15 - 16:00 Impulse for discussion, instant poll, discussion and wrap-up by chair

16:00 - 16:25 - Coffee break

Session 2: Software deployment
Chair: Volker Eyert (Materials Design, France)

16:25 - 16:30 Introduction and focus by session chair
16:30 - 17:00 Beatrice Carasi - COMSOL (Italy)
   Standard and advanced material modelling with COMSOL Multiphysics
17:00 - 17:30 Umberto Martinez - Synopsys (Denmark)
   Lean and agile software development of the QuantumATK platform
17:30 - 18:00 Gabriele Mogni - Exabyte.io (US)
   Cloud computing for Materials Modeling
18:00 - 18:45 Impulse for discussion, instant poll, discussion and wrap-up by chair
Tuesday 9 July 2019

Session 3: Economic impact of materials modelling
Chair: Donna Dykeman (ANSYS, UK)

08:55 - 09:00 Introduction and focus by session chair

09:00 - 09:30 Glenn Jones - Johnson Matthey (UK)
Economic Impact of Materials Modelling in R&D: There is clearly value, but we are still some way from a quantitative measure

09:30 - 10:00 Emilio Paolucci - Politecnico di Torino (Italy)
University – Industry Collaboration in an innovative context: A discussion of inhibitors and enablers

10:00 - 10:30 Sophie Snook - ANSYS (France)
Democratization of Modelling, Simulation and Information

10:30 - 11:00 Coffee break

11:00 - 11:30 Malgorzata Celuch - QWED (Poland)
Why set up a modelling SME when you are student? The economic impact of QuickWave software

11:30 - 12:15 Impulse for discussion, instant poll, discussion and wrap-up by chair

12:15 - 13:55 Lunch + Networking & Showcases

Session 4: Translation & Training for companies
Chair: Pietro Asinari (Politecnico di Torino, Italy)

13:55 - 14:00 Introduction and focus by session chair

14:00 - 14:30 Peter Klein - Fraunhofer (Germany)
Translation and Training from a SMEs perspective

14:30 - 15:00 Fedor Goumans - Software for Chemistry & Materials (Netherlands)
Making new material modeling techniques technology ready & pragmatic

15:00 - 15:30 Andre Haufe - DYNAmore GmbH (Germany)
On identification of industrial needs, providing of solutions and training of clients in macroscopic constitutive modelling in engineering applications

15:30 - 16:00 Coffee break

16:00 - 16:30 Svenn Halvorsen - NORCE (Norway)
Model Translator – What Is Required?

16:30 - 17:15 Impulse for discussion, instant poll, discussion and wrap-up by chair

17:15 - 18:00 Poster session (mini-presentations, 1 min)

20:00 - Conference dinner at the restaurant La Badessa
Wednesday 10 July 2019

Session 5: Interoperability & integration
Chair: Gerhard Goldbeck (Goldbeck Consulting, UK)

08:55 - 09:00 Introduction and focus by session chair

09:00 - 09:45 Gerhard Goldbeck & Jesper Friis - Goldbeck Consulting (UK) & SINTEF (Norway)
*EMMO: A semantic knowledge framework for materials and modelling*

09:45 - 10:15 Piotr Maciol - AGH University of Science and Technology (Poland)
*The prototype ontology for metal alloys*

**10:15 - 10:20 Poster Cup (best poster poll)**

10:20 - 10:45 Coffee break

10:45 - 11:15 Ian Bruno - Cambridge Crystallographic Data Centre (UK)
*Achieving Interoperability between Crystallography and Chemistry*

11:15 - 12:00 Impulse for discussion, instant poll, discussion and wrap-up by chair

**12:00 - 12:55 Lunch**

Session 6: Artificial intelligence & Industry 4.0
Chair: Eliodoro Chiavazzo (Politecnico di Torino, Italy)

12:55 - 13:00 Introduction and focus by session chair

13:00 - 13:30 Salvador Izquierdo - ITAINNOVA (Spain)
*Translation of physically-informed data-driven models of material transformation processes*

13:30 - 14:00 Haoyan Huo - University of California Berkeley (US)
*Data-mining millions of scientific literature for predictive materials synthesis*

14:00 - 14:30 Rajat Srivastava - Politecnico di Torino (Italy)
*Thermal properties of nanomaterials predicted through atomistic-to-continuum models supported by machine learning*

14:30 - 15:15 Impulse for discussion, instant poll, discussion and wrap-up by chair

**15:15 - 15:30 Final wrap up, conclusions and closing**
PRESENTATIONS ABSTRACTS

- **S1A**: Elisa Molinari - Designing materials with HPC: the MaX European Centre
- **S1B**: Arnulf Latz - Spatially resolved modeling and simulation of degradation in Lithium-ion batteries
- **S1C**: Vladimir Lobaskin - Multiscale modelling of bionano interface
- **S1D**: Ilian Todorov - DL_MESO: The UK’s DPD Vehicle for Academic and Industrial Collaboration
- **S2A**: Beatrice Carasi - Standard and advanced material modelling with COMSOL Multiphysics
- **S2B**: Umberto Martinez - Lean and agile software development of the QuantumATK platform
- **S2C**: Gabriele Mogni - Cloud computing for Materials Modeling
- **S3A**: Glenn Jones - Economic Impact of Materials Modelling in R&D: There is clearly value, but we are still some way from a quantitative measure
- **S3B**: Emilio Paolucci - University – Industry Collaboration in an innovative context: A discussion of inhibitors and enablers
- **S3C**: Sophie Snook - Democratization of Modelling, Simulation and Information
- **S3D**: Malgorzata Celuch - Why set up a modelling SME when you are student? The economic impact of QuickWave software
- **S4A**: Peter Klein - Translation and Training from a SMEs perspective
- **S4B**: Fedor Goumans - Making new material modeling techniques technology ready & pragmatic
- **S4C**: André Haufe - On identification of industrial needs, providing of solutions and training of clients in macroscopic constitutive modelling in engineering applications
- **S4D**: Svenn Halvorsen - Model Translator – What Is Required?
- **S5A**: Gerhard Goldbeck & Jesper Friis - EMMO: A semantic knowledge framework for materials and modelling
- **S5B**: Piotr Macioł - The prototype ontology for metal alloys
- **S5C**: Ian Bruno - Achieving Interoperability between Crystallography and Chemistry
- **S6A**: Salvador Izquierdo - Translation of physically-informed data-driven models of material transformation processes
- **S6B**: Haoyan Huo - Data-mining millions of scientific literature for predictive materials synthesis
- **S6C**: Rajat Srivastava - Thermal properties of nanomaterials predicted through atomistic-to-continuum models supported by machine learning
Designing materials with HPC: The MaX European Centre

Elisa Molinari

CNR-NANO and Department of Physics, University of Modena and Reggio Emilia (Italy)
Spatially resolved modeling and simulation of degradation in Lithium ion batteries

Latz Arnulf\(^1,2,3\)

\(^1\) German Aerospace Center, Stuttgart, Germany
\(^2\) Helmholtz Institute Ulm, Ulm, Germany
\(^3\) University Ulm, Institute of Electrochemistry, Ulm, Germany

Abstract
SEI growth and Lithium plating are two of the most important aging and degradation mechanisms in Lithium ion batteries. In both cases the development of a mesoscopic structure is initiated on atomistic scale via electrochemical and chemical reactions at the interface of anode and electrolyte and continues to grow into a nanoscale structure. The growth is mediated by a complex interplay of reactions and transport mechanisms. The evolved structures change decisively the local electrochemical environment at the interface and have influence on the macroscopic behavior and functionality of the battery. A thorough understanding of these multiscale processes in batteries requires going beyond an atomistic description on one side and a pure macroscopic porous electrode modeling on the other side. In our contribution, new theoretical models for SEI growth [1-4] and 3D structure resolved simulations of Lithium plating [5-6] are presented.

References
Multiscale modelling of bionano interface

David Power¹, Ian Rouse¹, Stefano Poggio¹, Erik Brandt², Alexander Lyubartsev², Vladimir Lobaskin¹

¹School of Physics, University College Dublin, Dublin 4, Ireland

Abstract

In biomedical and food technologies, the functionality of engineered materials and their biocompatibility are controlled by molecular-level interactions at the bionano interface, the nanoscale layer where biological fluids meet the foreign substances. We propose a systematic multiscale bottom-up method to coarse-grain the interactions of foreign materials with biological fluids [1,2]. Biomolecules (lipids, proteins and carbohydrates) are coarse-grained by mapping their main chemical fragments onto mesoscale beads, and their interaction with the substrate surface is characterised by potentials of mean force (PMF) from atomistic simulations. The substrate is represented by a two-layer model where the surface interacts with the molecule beads via those PMFs, while the core interacts with via van der Waals forces. The united-atom model for biomaterial-biomolecule segment interaction is used to evaluate the adsorption free energy of arbitrary biomolecules on a specified foreign surface and rank the molecules by adsorption affinity.

References

DL_MESO: The UK’s DPD Vehicle for Academic and Industrial Collaboration

Ilian Todorov and Michael Seaton

Science and Technology Facilities Council, UK Research and Innovation
Daresbury Laboratory, Warrington WA4 4AD, United Kingdom

Abstract

DL_Software is the Daresbury Laboratory ecosystem for molecular simulation methods. It provides for multiscale research via a QM/MM environment (ChemShell) [1] with MD (DL_POLY) [2] and MC (DL_MONTE) [3] modelling packages, advanced FF set-up program (DL_FIELD) [4] and access to the mesoscopic & continuum scales via the DL_MESO package. DL_MESO is a versatile, general purpose package for DPD and LBE simulation [5]. Not only is DL_MESO supported by UK’s communities such as CCP5 and UKCOMES, but it is a community code and software component respectively for the Horizon 2020 European HPC Centre of Excellence (E-CAM) [6] and Virtual Materials Market Place (VIMMP) [7].

The DPD package in DL_MESO offers a wide selection of functionality with a variety of ensembles and complementary tools, allowing for on-the-flight set-up and post-processing analytics. The package has been the “working horse” for the Computer Aided Formulation (CAF) project, a collaboration at STFC that has established long-standing partnerships with IBM and a range of consumer chemistry industries such as Unilever, GSK, DOW and Syngenta. The talk will give an overview of DL_MESO’s DPD capability and the general types of research carried out at CAF since 2010.

References

Abstract
The need of correct understanding and mathematical description of material behavior is critical with respect to obtain reliable results through simulation and gain significant industrial advantage.

In this session we will explore the need of using and developing tools for:

- Complex material descriptions, nonlinearity and interactions with the environment (multiphysics);
- Advanced mathematical tools for describing constitutive relationships and ad hoc numerical discretization (Equation based modeling, external library, thin structures and extra dimension);
- Multiscale modeling, homogenization and equivalent materials;
- Best use of experimental data (optimization and curve fitting);
- Process simulation (phase change\additive manufacturing).

Our continuous development in combining experimental testing and computer design is of paramount importance for manufacturing products that are up to our need for reliability, sustainability, performance and innovation (IoT, digital twins, portable apps).
Lean and agile software development of the QuantumATK platform

Umberto Martinez, Kurt Stokbro

Synopsys Denmark
Fruebjergvej 3, 2100 Copenhagen, Denmark

Abstract
QuantumATK, an integrated platform of electronic and atomic-scale modelling tools [1,2], is developed and deployed using modern lean, agile and scrum development methodologies. During this talk we will describe how the QuantumATK Team in Synopsys ensures that state-of-the-art commercial software is deployed to its customers while keep innovating. Testing, verification, validation, robustness, documentation, and support will be discussed.

References
Abstract
Materials development presently adopts an ever-increasing number of interdisciplinary computational approaches versed in modeling from physics-based or, lately, machine learning perspectives. Due to their complexity and the lack of standards, however, these approaches are yet to be made available to the majority of the scientifically capable population. Next-generation digital approaches are required in order to improve the impact of materials modeling and unlock the value of prior work [1].

Cloud computing today serves as the focal point for the digitalization efforts in a vast majority of organizations globally, both enterprise, academic and/or governmental. Apart from the computational aspect, the cloud serves as the uniform foundation for collaborative efforts on a global scale, allowing to build accessible, and interoperable infrastructure for data-centric and repeatable digital research practices.

The presentation will focus on the role of cloud computing in materials development [1], demonstration of its capabilities [2, 3] and future outlook.

References
Economic Impact of Materials Modelling in R&D: There is clearly value, but we are still some way from a quantitative measure

Glenn Jones¹

Johnson Matthey Technology Centre, Blounts Court, Sonning Common, Reading, RG4 9NH, UK

Abstract
This talk will set the scene of how materials modelling is delivering value within the industrial setting. With a particular focus on the atomic-scale and its deployment in materials product development.

As our research groups deliver value, raise in profile and ultimately grow, it becomes increasingly important to document the value delivered; especially if one aspires to a higher maturity level.

There are a range of complex settings in which materials modelling is but one of a number of improvements to factors influencing the product development process (or more broadly speaking R&D).

Following a general discussion on the above, the talk will culminate in highlighting the difficulties of formulating a quantitative value measure, with a view to stimulating discussion on, how we might, in the future.
University – Industry Collaboration in an innovative context: A discussion of inhibitors and enablers
Emilio Paolucci, Simona Calà
Department of Management and Production Engineering, Politecnico di Torino

Abstract

In the context of Materials Modeling, new forms of University-Industry collaboration can act as an accelerator of the innovation process. Such collaboration is very complex due to the presence of various types of “inhibitors” (technical, communication, economic and relational). Inhibitors include a variety of factors that block or delay the commercialization of results of research.

The focus of the presentation will be twofold. On one side, it will discuss the characteristics of such inhibitors. On the other one, it will address possible enablers aimed at mitigating their effects and facilitate transfer of knowledge from research to industry.

The discussion about enablers will focus on two specific aspects. The first one regards the need to create a “shared” language and coordination networks to manage information exchanges. “Translators” can contribute to this aspect, by helping transform academic discoveries into practical requests from companies and vice versa. The second aspect reflects the need to make companies aware of their strengths and weaknesses. In this direction, the Maturity Model may help companies identify areas of intervention and related investments needed to produce the required outcomes. It also plays a key role in helping create a map of the “as is” and “to be” situations, developing awareness in organizations on the basis of four fundamental pillars: people, processes, data and tools, each of these at different "maturity" levels. Please refer to [1,2] for related material.

References
Abstract
It is well accepted that 80% of product life cycle costs are locked in at the ideation, or concept, phase during which materials and processes are selected for a design. This phase is critical to unlocking market opportunities and greatly influences time-to-market. Modelling and simulation can significantly impact this life cycle phase, but common barriers to adoption still exist such as steep learning curves, design complexity, long time-to-solution, inaccessible tools and data. In this talk we demonstrate how the democratization of tools and information at the continuum scale have improved the adoption of modelling and simulation across a wider end-user spectrum and improved economic returns on investment.
Why set up a modelling SME when you are student? The economic impact of QuickWave software
Malgorzata Celuch
QWED Sp. z o.o.

Abstract

“An entrepreneur knows that setting up in business is a risk. They need a robust business plan (..) and competitor analysis and a good knowledge of the market.” [1] - I knew none of this, when I was a Ph.D. student - or more precisely, a student on a maternity leave. When my studies on electromagnetic modelling methods [2] began to contradict the then-established dogmata, and journal submissions were hindered by never-ending reviews, my supervisor suggested proving our concepts on the market. The delayed paper [3] was published when a beta-version of QuickWave was already being tested at four universities, and in 1997 we founded QWED to supervise its further commercial developments. This talk will present selected (non-confidential) examples of how QuickWave modelling has impacted:

1. QWED (www.qwed.eu) - grown first on licence sales, and then also on software-based consulting and measurements; now a company of 10 persons successfully competing with corporations of 10 thousand in the field of EM simulations and material test fixtures;
2. our projects, from Eureka E!2602 [4] to the on-going H2020 MMAMA [5];
3. our partners in material research, from improving the safety of reheated frozen foods [4] to reducing the energy consumption in mineral rock comminution [6];
4. our first users in US space labs, who became our great marketing force by publishing their QuickWave results in such famous project as the Atacama Large Millimeter Array [7];
5. our industrial customers, e.g. a leading supplier of domestic microwave ovens, who found QuickWave “not only as the best but also very significantly better than the contenders” and reported “a drastic improvement in our possibilities to model the whole microwave system”.

I focus on bilaterally coupled EM-thermal modelling of materials [8], which distinguishes QuickWave from its competitors on the EM simulations market. QWED seeks collaborations to develop new materials models for QuickWave, enhancing its industrial relevance.

References

Session 4A

Translation and Training from a SMEs perspective

Peter Klein

Fraunhofer ITWM, Kaiserslautern, Germany

Abstract
The EMMC-CSA has spent great efforts in defining concepts like Business Decision Support Systems BDSS, Key Performance Indicators KPI and Translation methodologies. In particular, a Translators Guide [1] had been published with the aim to streamline Translation processes. Picking up these definitions, experience in a running EU project, FORCE [2], and as a solution architect at Fraunhofer ITWM, helped to identify a set of necessary skills from a practical point of view which are necessary for effective Translation processes applied to challenges faced by SMEs.
In this presentation, an Agile Translation Process, Fig. 1, will be presented. Supporting tools and necessary Translators skills are identified; in particular how to train industrial users from SMEs in using these tools in their daily work. From this point of view, a way to train Translators will be proposed.

Figures

Fig.1: Agile interpretation of the EMMC-CSA Translation process

References
Session 4B

Making new material modeling techniques technology ready & pragmatic

Fedor Goumans

Software for Chemistry & Materials, Amsterdam, The Netherlands

Abstract

New computational techniques from academia which can be promising for driving RD&I are usually not easy to adapt as industry-ready solutions. Especially companies with small modeling teams do not have the time to adapt novel techniques which do not work out of the box, while companies with larger modeling teams often also benefit from a shorter time to solution with easy to deploy software.

At SCM we work on implementing new capabilities both in-house, and in collaboration with academic and industrial partners. SCM focuses on software development and does not do consultancy, which means that to catalyze industrial adoption oftentimes case studies are key. We will demonstrate this with a few case studies on organic electronic materials, sputtering deposition and we'll highlight the recently started EU-funded effort to assimilate commercial and academic software in a single multi-scale modeling platform for chemical reactors, ReaxPro, in collaboration with industrial end users.
On identification of industrial needs, providing of solutions and training of clients in macroscopic constitutive modelling in engineering applications

Andre Haufe\textsuperscript{1} & Paul DuBois\textsuperscript{2}

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\textsuperscript{2}Consultant, 45529 Pebble Beach Court, Northville, MI 48168, USA

Abstract
In recent years the complexity of new material development, its application in industrial design and production environment was ever increased. All steps along this line have been strengthened continuously with the help of new computer-based modelling techniques as well as advanced numerical schemes which are getting closer and closer to capture the real physics for all the many applications targeted. While many of these new techniques cannot hide their complex nature even from the educated eye, one would expect that within the community that applies some of most matured and most applied techniques, namely the finite element method in spatial and temporal discretization of mechanical problems, should long have established methods to collect and solve problems as well as disseminate the solutions, and train stakeholders along the value chain. However, the latter should be questioned.

The present contribution exemplifies the aforementioned statement along the development of new macroscopic constitutive models for two material classes namely steel and polymers. It will be shown that the process of collecting challenges from clients, identification of issues with existing models or integration newly acquired test data will eventually trigger the decision process to enhance existing models or develop completely new approaches in engineering simulation applications. It will be shown that this process is often not plannable ahead nor it follows a standard process. Furthermore, the complexity of the subject leaves the typical product designer or CAE engineer behind. Dissemination and training of these new methods that incorporates development, implementation and verification, calibration and validation, is therefore of uttermost importance [1].

References
Abstract

The task of a model translator is to bridge the gap between mathematical modelling and real-life industrial problems. Sound competence from two “different worlds” is required: Proper understanding of the industrial business case and good modelling knowledge. The translator needs to understand the “tribal language” and the culture in both domains, which can be really challenging.

Translator training should be aimed at filling the relevant gaps, depending on the translator’s background. He cannot possibly be an expert in all fields. Hence, it is important that he also:

- Knows his limitations
- Knows where to find help/assistance

Further, the translator will need:

- Good communication skills
  - Active listening and questioning techniques to
    - Enable proper understanding of the client’s need and wishes
  - Presentation skills to present
    - A model solution/proposal in the “client’s language”
    - Modelling results that are understandable, reliable and usable for the client
- Integrity – the client’s needs is priority number one!

References

EMMC Workshop 2019
Industrial Impact of Materials Modelling
8-10 July 2019, Turin - Italy

Session 5A

EMMO: A semantic knowledge framework for materials and modelling

Gerhard Goldbeck¹ & Jesper Friis²

¹ Goldbeck Consulting (UK)
² SINTEF (Norway)

Abstract

An introduction to the European Materials & Modelling Ontology (EMMO) will be given. It provides a framework to integrate materials data and models into a coherent, science-based knowledge system, enabling interoperability and enhanced decision making based on a combination of data (statistics) and reasoning (logics). An interoperability example from the field of multiscale modelling will be given.
Abstract
The European Material Modelling Ontology (EMMO) has been designed as a base for a common language for describing of numerical models of materials. However, relatively high abstraction level requires developing of customized ontologies for particular domains. In this talk a prototype of an ontology, consistent with EMMO, dedicated for representing of metal alloys is presented. It was designed to support interoperability of several numerical models used in multiscale modelling of precipitation kinetics in aluminium alloys [1].
A main challenge was approaching the problem of effective description of metal alloy. On the one hand, mereotopological approach represented by EMMO had to be followed. On the other hand, a material state in metal processing community is based on distinguishing of particular grains. Furthermore, granularity of a description is not straightforward. In this talk, contradictory requirements are discussed, and preliminary solutions are proposed.

References
Session 5C

Achieving Interoperability between Crystallography and Chemistry

Ian Bruno

The Cambridge Crystallographic Data Centre, Cambridge UK

Abstract
The criteria for interoperability set out in the FAIR Data Principles highlight the need for standard formats for knowledge representation and associated vocabularies. Within the domain of crystallography, the Crystallographic Information File (CIF) largely satisfies these requirements by enabling semantic representation of many facets of a diffraction experiment. Another aspect of interoperability is the ability to reference between data resources. Here, standard identifiers are key and the IUPAC International Chemistry Identifier (InChI) is an important enabler of links to chemical data resources. Knowledge representation within the domain of chemistry is aided by the many terminologies have been developed by IUPAC over the years along with a range of formal and de facto standard formats for representing chemical structures and spectra. This presentation will describe the components that enable interoperability of crystallographic and chemical data and activities aimed at enhancing these and their adoption.
Session 6A

Translation of physically-informed data-driven models of material transformation processes

Salvador Izquierdo, Valentina Zambrano, Rafael Rodríguez

Multiphysics & Multiscale Simulation Group
Instituto Tecnológico de Aragón (ITAINNOVA), Zaragoza, Spain

Abstract

Within the Industry 4.0 context, the main challenges for achieving a goal of zero-defect manufacturing are: the design of fast and reliable start-ups, the design of optimal control strategies and the management of uncertainty. We introduce a methodology (CAELIA) to systematically approach the solution of these challenges. CAELIA is a Computer-Aided-Engineering (CAE) management Library for building Intelligent Applications in the context of Advance Manufacturing and Integrated Computational Material Engineering (ICME). It is designed to shorten the time needed to build a prescriptive Digital Twin of a system and to enable its efficient lab or shop-floor deployment as a cyberphysical system. The general approach is to develop models based on simulations and/or data but preserving the physical meaning of the processes allowing interpretability of the actions taken when using these models. The core algorithm of the main library within CAELIA is an in-house developed tensor factorization for sparse and unstructured data.

CAELIA, as a methodology, has been designed for allowing Open Innovation between academia, translators and end-users. Our current experience deploying CAELIA will be detailed. This include: a discussion about two success cases applications in extrusion and injection processes; CAELIA as a Roadmap; training needed along the tier of model building, deploying and consuming; and a discussion of best practices for translation.

References

[1] https://github.com/caeliaITAINNOVA
Session 6B

Data-mining millions of scientific literature for predictive materials synthesis

Haoyan Huo\textsuperscript{1,2}, Olga Kononova\textsuperscript{1}, Tanjin He\textsuperscript{1}, Wenhao Sun\textsuperscript{2}, Ziqin Rong\textsuperscript{2}, Gerbrand Ceder\textsuperscript{1,2}

\textsuperscript{1} Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA
\textsuperscript{2} Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Abstract

In the past thirty years, materials designing had been significantly accelerated by high-throughput computation methods and large-scale computed materials databases. However, the materials discovery pipeline remains bottlenecked by the difficulty of experimental materials fabrication, which still requires months or even years of trial-and-error to successfully synthesize a target compound. To facilitate the materials synthesis problem, we developed a data-mining pipeline that extracts inorganic materials synthesis information from nearly four million of available online scientific publications, using natural language processing and text-mining techniques. Especially, we have generated an automatically extracted dataset consisting of 19,477 solid-state synthesis reactions. Attributes in this dataset include starting materials, target compounds, experimental operations, and detailed synthesis conditions and parameters. Using this codified synthesis information, machine learning and materials informatics are applied to analyze features of materials synthesis experiments. Our methods allow us to mine the synthesis knowledge locked-up in written natural language to achieve data-driven synthesis prediction for next-generation materials discovery and fabrication.

Figures
Thermal properties of nanomaterials predicted through atomistic-to-continuum models supported by machine learning

Matteo Fasano, Rajat Srivastava, Annalisa Cardellini, Eliodoro Chiavazzo, Pietro Asinari
Department of Energy, Politecnico di Torino - Italy

Abstract
The enhanced thermal properties of nanomaterials are exploited in many fields, from aerospace to electronics industries, from automotive to biomedical applications. Nevertheless, these properties are determined by phenomena spanning from the nano to the macro scale and, thus, should be simulated by tailored multi-scale techniques. In this presentation, the original multi-scale materials modelling approach to the thermal transport through nanomaterials developed at the Multi-Scale Modelling Laboratory (www.polito.it/small) and the employed high-performance computing resources will be presented. The focus will be on predicting the thermal conductivity of nanocomposites (epoxy matrix + carbon nanofillers) using fast mesoscopic models, whose input parameters come from both atomistic models (interface properties) and continuum models aided by machine learning (macroscopic corrections). The presented models, which have been both verified against commercial software and validated against experiments, may provide guidelines towards the technical-economical optimization of novel nanostructured materials with tunable thermal properties. This work has received funding from the European Union’s Horizon 2020 research and innovation program MODCOMP under grant agreement N. 685844.
POSTER ABSTRACTS

1. Cinzia Giannini - X-ray MicroImaging Laboratory (XMI-L@b)
2. Cinzia Giannini - SUNBIM: a package for X-ray imaging of nanomaterials and biomaterials using SAXS, WAXS, GISAXS and GIWAXS techniques
3. Javier Gomez - A machine learning application to mechanical and fracture material characterization
4. Martin Thomas Horsch - Molecular model database of the Boltzmann-Zuse Society for Computational Molecular Engineering
5. Amaya Igartua - Modelling activities as a tool to optimize materials, products, process and performance
6. Otello Maria Roscioni - A Reversible Coarse Graining Model for Organic Functional Materials
7. Fabio Sacconi - TiberCAD: a tool for multiscale simulation of nanostructured devices
8. Massimo Celino - EoCoE: the European Energy oriented Centre of Excellence
9. Lorenzo Chiavarini - iMat: Data extraction from scientific papers through Machine Learning
10. Paolo De Angelis - Exploring the free energy landscapes to predict surfactant adsorption isotherms at solid-liquid nanoscale interface
11. Silvia Chiacchiera - Explicitly polarisable mesoscale (DPD) models for water
12. Malgorzata Celuch - QuickWave conformal FDTD modelling: electromagnetics and beyond
13. Gabriele Falciani - Multi-scale modelling of transport phenomena through engineered soap films for fuel generation
14. Xavier Alvarez - Multiscale model for thermal transport at the nanoscale: From ab-initio to Finite Elements description
X-ray MicroImaging Laboratory (XMI-L@b)

D. Altamura, L. De Caro, C. Giannini, M. Ladisa, R. Lassandro,
F. Scattarella, T. Sibillano, D. Siliqi, A. Terzi

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Abstract
X-ray Micro-Imaging Laboratory (XMI-L@b): facility with a scanning microscope in which a beam of hard X-rays (8KeV), focused down to 70µm, illuminates a sample area, whereas an area detector placed at an appropriate distance records the signal diffracted/scattered, in the low scattering angle (SAXS), from each illuminated spot. At the end of the collection, the measurements are recomposed together by extracting from them, through specific crystallographic and statistical approaches, quantitative information to measure variations of one of the structural components of the sample at the nanoscale. A photodiode records the transmitted intensity, also providing a contrast absorption microscopy. It is also possible to collect low and high scattering angle data in transmission (SAXS / WAXS) or in reflection (GISAXS / GIWAXS). It is used for analysis at the molecular and atomic scale of fabrics, natural or engineered thin films, nanostructured surfaces, nanomaterials and biomaterials.

References
**SUNBIM: a package for X-ray imaging of nanomaterials and biomaterials using SAXS, WAXS, GISAXS and GIWAXS techniques**


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**Abstract**

SUNBIM (Supramolecular and submolecular nano- and biomaterials X-ray imaging) is a suite of integrated programs which, through a user-friendly graphical user interface, are optimized to perform the following:

- **q-scale calibration and two-dimensional-one-dimensional folding on small- and wide-angle X-ray scattering (SAXS/WAXS) and grazing-incidence SAXS/ WAXS (GISAXS/GIWAXS) data, also including possible eccentricity corrections for WAXS/GIWAXS data**
- **background evaluation and subtraction, denoising, and deconvolution of the primary beam angular divergence on SAXS/GISAXS profiles**
- **indexing of two-dimensional GISAXS frames and extraction of one-dimensional GISAXS profiles along specific cuts**
- **scanning microscopy in absorption and SAXS contrast.**

The latter includes collection of transmission and SAXS data, respectively, in a mesh across a mm² area, organization of the as-collected data into a single composite image of transmission values or two-dimensional SAXS frames, analysis of the composed data to derive the absorption map and/or the spatial distribution, and orientation of nanoscale structures over the scanned area.

**References**


A machine learning application to mechanical and fracture material characterization

F.J. Gomez¹, M. Ispizua¹, M.A. Martín-Rengel², J. Ruiz-Hervías²

¹ ADVANCED MATERIAL SIMULATION SL, Bilbao, Spain
² Materials Science Department, Polytechnic University of Madrid, Spain

Abstract
Industrial and manufacturing processes, as rolling, extrusion, forging, drawing, coating... modify material properties. Mechanical and fracture magnitudes of the final product are different than raw material. In situ material characterization is a challenge task to know the real material properties of a product in its final state in components which arbitrary shape does not permit a conventional characterization.

A strategy of non-conventional tests combined with numerical simulation and machine learning techniques is proposed. The basic idea is to determine with machine learning the mechanical or fracture material properties that introducing in numerical simulation reproduces better the experimental tests. This technique is a specific procedure for obtaining material functions as the plastic stress strain curve in continuum analysis or the softening curve in fracture.

The same inverse machine learning algorithm has been applied to different test and different magnitudes: ring compression test and spheric nanoidentation to determine the plastic stress-strain curve and three point bending test to obtain the softening curve in concrete.

References
Molecular model database of the Boltzmann-Zuse Society for Computational Molecular Engineering

Simon Stephan,¹ Hans Hasse,¹ Martin Thomas Horsch,² Jadran Vrabec³

¹Technische Universität Kaiserslautern, Laboratory of Engineering Thermodynamics, Erwin-Schrödinger-Str. 44, 67663 Kaiserslautern, Germany
²UK Research and Innovation, STFC Daresbury Laboratory, Keckwick Ln, Daresbury, Cheshire WA4 4AD, United Kingdom
³Technische Universität Berlin, Thermodynamics and Process Engineering, Str. des 17. Juni 135, 10623 Berlin, Germany

Abstract
The openly accessible molecular model database (MolMod DB) of the Boltzmann-Zuse Society for Computational Molecular Engineering contains materials relations (force fields) for over 150 low-molecular fluids, meant for molecular modelling and simulation with molecular dynamics (MD) and Monte Carlo (MC) solvers [1]. The molecular models in the database have been published in about 30 articles over the past 20 years, which are associated with the respective entries and can be followed on the MolMod DB web front end.

The database provides a wide range of search functionalities, e.g., for substances (names and CAS numbers) and model classes. Input files for several common environments can be downloaded via the web front end [2], including the file formats used by the molecular simulation codes ms2, GROMACS, LAMMPS, and ls1 mardyn. The standardization efforts guided by the EMMC will create an opportunity to integrate modelling algorithms and tools with repositories, open translation environments, and virtual marketplaces.

Accordingly, the MolMod DB is intended to be interoperable with infrastructure associated with the EMMC, including the Virtual Materials Marketplace (VIMMP); Acknowledgment: This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 760907.

References
Modelling activities as a tool to optimize materials, products, process and performance

Dr. Amaya Igartua, Dr. Borja Zabala, Dr. Borja Coto, Dr. Cristina Monteserín, Itxaso Gascón, Jon Lambarri, Aitor Fernandez

Abstract
In the paper it is described the need of modelling to optimize different materials, products, process and performance:

- Molecular Dynamic and Atomistic modelling is used to predict properties at the nanoscale (eg. Nanocomposites and nanopigments) by Borja Coto (borja.coto@tekniker.es). Doctoral Thesis
- Piezoelectric simulation has been used for product (nebulizer) design by Jon Lambarri (jon.Lambarri@tekniker.es)
- Optimization of laser and curing processing by modelling (Jon Lambarri, and Cristina Monteserin (cristina.monteserin@tekniker.es), Doctoral Thesis.
- Machining models to improve the process, reduce the experimental set-up and New tool geometries to reduce manufacturing errors by Itxaso Cascón (ltxaso.gascon@tekniker.es)
- Use FEM tools to predict failure modes analytically and define tribological tests by Aitor Fernandez (aitor.fernandez@tekniker.es)
- Prediction failure modes lifetime: constructing innovative equipment's, reproducing wear mechanisms, building lifetime equations from experimental data by Borja Zabala (Borja.zabala@tekniker.es; Doctoral Thesis)

References
Poster 6

A Reversible Coarse Graining Model for Organic Functional Materials

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Abstract

A new Coarse Grained (CG) modelling approach is presented, where complex organic molecules are modelled in terms of connected ellipsoidal beads. The CG model aims at reproducing realistically large scale morphologies (e.g. up to 100 nm thick films) for the materials involved, while being able to generate, with a back-mapping procedure, atomistic coordinates suitable, with limited effort, to be applied for charge transport calculations. Detailed methodology and an application to the common hole transporter material α-NPD is provided.

Comparison between the atomistic and coarse-grained representations of the molecule α-NPD.

References

Poster 7

TiberCAD: a tool for multiscale simulation of nanostructured devices

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Abstract

We present tiberCAD\(^1\), a multiscale software tool for CAD/CAE applications in the field of electronic and optoelectronic nanostructured devices. It allows to model and design innovative devices based on new materials, such as nitrides quantum well-based LEDs\(^2\), nanowire FETs, organic and hybrid solar cells, for applications in lighting, sensors, energy harvesting. tiberCAD provides both atomistic (DFT, ETB, NEGF) and FEM-based tools (EFA quantum, elasticity, thermal, particle transport) to accomplish the critical requirements imposed by the recent developments in Key Enabling Technologies such as micro-nanoelectronics, nanotechnology, photonics and advanced materials, considered central for innovation and market growth.

Fig.1: Projection of atomistic quantities (VFF strain, quantum charge) onto a FEM grid for multiscale modelling.

References


Abstract

The new European roadmap in HPC (High Performance Computing) foresees a new generation of supercomputers that are capable of deliver a computational power in the range of exascale. Exascale means that 1018 floating point operations per second could be performed at the same time on the same challenging application. The availability of this tremendous computational power opens new ways to face challenges in research. Materials science will be greatly affected since a new kind of dynamics between theory and experiment will be established with the potential to accelerate materials discovery to meet the increased demand for task-specific materials. New approaches will be enabled and new opportunities will be available to better face the heightened demand for automation, advanced analysis and predictive capabilities.

In the European sphere, the transversal multidisciplinary approach is the key ingredient of the Horizon2020 Energy oriented Centre of Excellence (EoCoE, www.eocoe.eu) which aims to accelerate the European transition to a reliable low carbon energy supply exploiting the ever-growing computational power of HPC. EoCoE is designed to contribute to this energy transition via targeted support to selected applications challenges that cover different domains of the renewable energy sector: water, wind, materials, meteorology and fusion. This support is provided by a powerful transversal and multidisciplinary basis that gathers the necessary HPC technical challenges: programming models, linear algebra, I/O data flow and ensemble runs. The final goal will be to share high performance computing expertises across the different fields and over time to accelerate their development at a lower cost and foster their scientific and economic impacts.
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iMat: Data extraction from scientific papers through Machine Learning

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Abstract

The rapid evolution of current technologies requires continuous development of novel and improved materials. In this view, data analysis is assuming everyday more and more importance. Materials data can be either generated via numerical simulations or retrieved from already available sources [1]. In both cases, a large amount of data must generally be treated. Therefore, efficient tools for (big) data mining are of paramount importance to extract emerging characteristics. In this sense, artificial intelligence offers several possibilities. In this project, iMat [2], we adopt Natural Language Processing (NLP) to extract materials data from literature papers. Based on IBM Watson apps, we developed an algorithm able to process articles pdfs and to automatically extract targeted information. Here we apply the algorithm to screen relevant properties for thermochemical heat storage in zeolite-water couples. Based on a sample training-validation set of pertinent scientific papers, which are retrieved using dedicated Springer-Nature APIs, we show that the algorithm is able to extract target properties very efficiently and in a semi-automatic way. These properties eventually provide new insights and possibility of further processing. With proper training-validation procedure, the developed algorithm can be easily applied for screening of other properties and analysis of different applications.

References

Poster 10

Exploring the free energy landscapes to predict surfactant adsorption isotherms at solid-liquid nanoscale interface

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Abstract
The long-lasting stability of nanoparticle (NP) suspensions in aqueous solution represents one of the main challenges in colloidal science. The addition of surfactants is generally adopted to increase the free energy barrier between NPs and hence to assure a more stable condition avoiding the NP sedimentation [1]. However, predicting the exact surfactant concentration enabling a well dispersion of NPs still encounters several challenges. In this poster, we show a molecular modeling-based approach to predict the adsorption isotherm of surfactants on bare alpha-alumina nanoparticles suspended in aqueous solution. First, Steered Molecular Dynamics (SMD) simulations are carried out to explore the free energy landscape (FEL) of the adsorption phenomena. Second, the minimum of the free energy is considered to compute the Langmuir Isotherm, and thus to calculate the quantity of adsorbed surfactants as a function of their concentration. In addition, the adsorption FELs are also investigated by tuning the percentage coverage of surfactants adsorbed on the nanoparticle surface. The results shed light on the competing effects of enthalpic and entropic contributions. Specifically, the adsorption is highly promoted by the tail-tail adhesion, while is prevented by the intense steric effects derived by the excluded volume phenomena and the hydration layer formation at solid-liquid interface. In conclusion, by synergistically blending Molecular Dynamics (MD) with the Langmuir theory we show how to extract the adsorption isotherm curves in the low surfactant concentration region. This model suggests some guidelines to rational design stable NP suspensions in aqueous solutions.

References
Explicitly polarisable mesoscale (DPD) models for water
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Abstract
Water is a polar liquid and has a dielectric permittivity much higher than typical apolar liquids, such as light oils. This strong dielectric contrast at water-oil interfaces affects electrostatics and is important, for example, to include these effects to describe biomolecular processes and water-oil mixtures involving surfactants, as detergents. This poster summarizes the work recently done in this direction within an E-CAM pilot project [1], developed in collaboration with Unilever and Manchester University. We have proposed and analysed a class of polarisable solvent models to be used in Dissipative Particle Dynamics (DPD) [2], a coarse-grained particle-based simulation method commonly used in various industrial sectors. Related software modules for the DL_MESO [3] package have also been developed and are briefly described.

References

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**Poster 12**

**QuickWave conformal FDTD modelling: electromagnetics and beyond**

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QuickWave software was launched onto the market in 1997, by a team of enthusiasts who believed it possible to induce microwave engineers to use computer modelling in place of simple but approximate design formulae, and to trust it as much as hardware prototyping. The software solves Maxwell equations with the in-house conformal FDTD method [1,2], which emulates the physical processes directly in the time domain (TD) and retains the numerical efficiency of the classical finite-difference (FD) approach, while approaching the geometrical fidelity of finite elements with natural immunity to spurious modes [2]. Different types of materials [3-6] and interfaces [7,8] are modelled, and coupling to thermal [9], kinetic [10] and optical [8] effects is provided. QWED team seeks collaborations to extend QuickWave system with the modelling of new media types and physical phenomena, to further proliferate the modelling in industry and increase its relevance to material science.

![Standard stair-case FDTD meshing versus conformal FDTD in QuickWave.](image1)

![Poynting vector distribution in a photonic crystal structure.](image2)

![Multiphysics modelling of enthalpy distribution in Whirlpool max oven.](image3)

References:


Poster 13

Multi-scale modelling of transport phenomena through engineered soap films for fuel generation

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Abstract

This work is part of the research activities foreseen in the recently funded SoFiA project [1], supported by the European Commission under the H2020-FETOPEN framework call (i.e. Future and Emerging Technologies Open). The overall project objective is the development of a demonstrator for artificial photosynthesis capable of converting CO2 into usable fuel and industrial feedstock by exploiting the unique structural properties of soap films and soap bubbles obtained by photocatalytic surfactant molecules.

More specifically, we envision a comprehensive multi-scale model of the photosynthetic process describing photo-electro-chemical reactions, species transport in liquid and gas phases, proton and electron transport within the soap-film based membrane. Here, we will focus on a preliminary continuum model including the transport of gaseous species through the soluble monolayers of a soap film assuming Fick’s diffusion, in line with previous studies [2]. Since the permeability of the surfactant layer depends on the surfactant itself [3], the above continuum model will be coupled with properly designed molecular dynamics simulations in order to accurately estimate all the necessary parameters. Initial simulations will focus on hexaethylene glycol monododecyl ether (C12E6) as a base surfactant at various levels below the critical micelle concentration. We have already initiated some classical molecular dynamics of Water-CO2 interfaces as well as those including the model surfactant. These simulations will allow us to build a molecular description of the packing of water, CO2 and surfactant molecules at the interface and further facilitate comparisons with the continuum models.

Figure 1: Multi-scale model of gas diffusion through the soap film

References

**Poster 14**

**Multiscale model for thermal transport at the nanoscale: From ab-initio to Finite Elements description**

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**Abstract**

The large reduction in the characteristic scale of electronic devices has derived in important problems related with heat management at the chip scale. Heat evolution at the nanoscale seems to be different from the Fourier’s law. New equations should be obtained in order to understand the physical reasons for this change of behaviour. Engineering tools should be upgraded with the new equations to include the new physics and help designers improve the thermal management capabilities in future electronic devices.

We propose a multiscale framework combining ab initio calculations, thermodynamic equations and finite elements modeling to describe thermal transport at these scales with remarkable predictability.
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