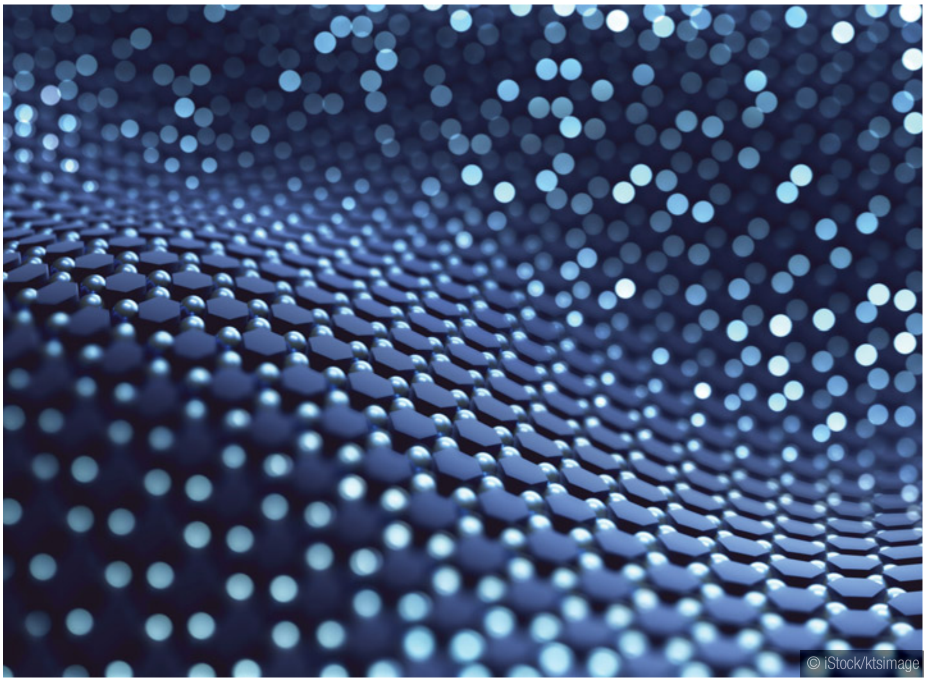
The European Materials Modelling Council's Chairwoman and EMMC CSA Project Co-ordinator, Dr Nadja Adamovic, tells *SciTech Europa Quarterly* about the work and role of the Council, as well as some of the challenges facing the wider incorporation of materials modelling in industry

Materials modelling – a key tool for industry

IT has been demonstrated in many individual cases that materials modelling is a key enabler of R&D efficiency and innovation. Companies reported that computational modelling benefits include reduced R&D time and cost, more efficient and targeted experimentation, more strategic approach to R&D, a route to performance optimisation, wider patent protection, improved supply chain control, enhanced decision making and early understanding of application performance aiding faster and more assured market introduction.

The European Materials Modelling Council is a co-ordination and support action which began in September 2016. As a three year project, it now has 16 project partners as well as a core group who perform the main actions of the project, which includes the organisation of a number of meetings and workshops, where the Council discusses relevant issues with both European and international stakeholders.

SciTech Europa Quarterly asked the EMMC's Chairwoman and EMMC CSA Project Co-ordinator, Dr Nadja Adamovic, about the work and role of the Council, as well as some of the challenges facing the wider incorporation of materials modelling in industry.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Despite several clear benefits, modelling today is still not always an essential part of or a critical tool in creative materials design or business decision making on product innovation. How is the EMMC working to change that? What are the biggest challenges here?

Industry argues that one of the key factors in use of materials modelling is their ability to trust the process and its results, as well as the quality of the modelling results and the speed with which they can obtain them in order to generate solutions to their problems.

Of course, these challenges are different in different application fields, and while some modelling techniques are being used in different industry areas, it is not yet at the point where we can say that this is a general trend, as the majority of industry sectors are still not exploiting materials modelling sufficiently.

When looking at the international level, Europe is very strong in the area of modelling development within academia; however, when it comes to the exploitation of these models and software tools, Europe is sometimes lagging behind other countries. Indeed, this is something that has been recognised amongst European stakeholders, and it was for this reason that the EMMC was first established, as we are working to bring the exploitation of materials modelling to industry and so speed up the lab-to-market process.

An integral part of this is identifying the shortcomings of the available models. That is, while there are many excellent models and techniques out there, there are, of course, others which require work and we are working to solve those issues. We do that by identifying any gaps and proposing ways for them to be filled – as we are not a research project we do not implement these measures ourselves; rather, we discuss them with the relevant stakeholders and then, within the EMMC roadmap, we propose what can be done to enhance exploitation.

What has been industry's feedback in terms of where these shortcomings are?

Based on feedback from industry, we have identified the most important shortcoming as

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being a lack of adequate models to simulate complex problems. Furthermore, from the industrial perspective there is also very often a lack of validation of both the available models and those models which are still in the development stage. This is extremely important for industry because they have to be able to be able to trust the models and to be able to know what they can achieve via the model in a quantifiable way. They also need to be able to understand the technical risks, and then, of course, as businesses they need to understand any inherent financial risks, too.

From the industrial perspective, some modelling tools are also not being used efficiently because they are quite difficult to use; or they may not be accurate enough; or the team may not be able to get answers to very specific questions in a timely manner. This therefore comes back to the issue of the shortcomings in the models and the ways they can be filled. What is more, technical challenges also remain with regard to developing predictive models.

The cost involved in incorporating materials modelling into SMEs is also often a barrier. Indeed, quite a significant investment is often required, at least in the beginning, and while larger companies are able to absorb this expense, smaller ones are not. This cost can either be in terms of paying to attract the right experts to use the modelling techniques, or in terms of the infrastructure needed to support such experts. Often, both are required, which can be expensive.

As such, before companies commit to investing in these areas they have to understand that by doing so they stand to begin making a profit from this within a certain timeframe, which is still very difficult to quantify. This difficulty stems, at least in part, from the fact that many companies which have already made these investments do not make their benefits public knowledge.

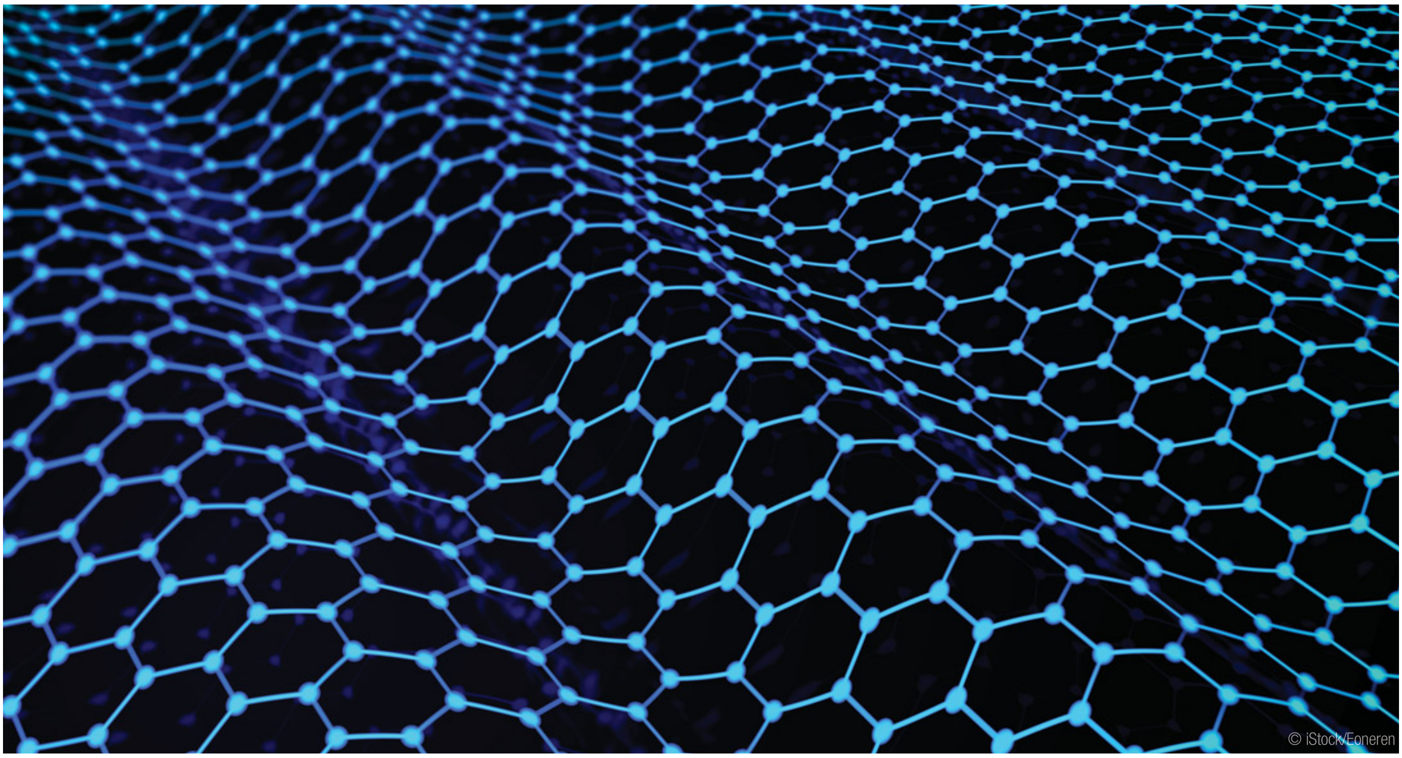
When we look at the numerical simulations being used in industry, continuum models based on structural mechanisms and computational fluid dynamics are typically being employed, and volume analysis within these models forms a part of the product lifecycle management, or computer-aided engineering process. This is now relatively mature (but there is potential for further developments here too) and so some data is available for this which can help inform the business decisions of others who may be considering investing in materials modelling.

This is a little different with regard to discrete modelling, where we are able to go into greater detail and explore material composition and structure. This requires other models and, typically, the models available here are not taken into count in product lifecycle management tools, meaning that there is a distinct lack of data which could be used to inform business decisions.

Are there known reasons as to why models are lacking in some areas or, perhaps, remain incomplete?

Software development takes 10-15 years before marketable software tools emerge. While Europe is strong with regard to this within academia, there are a number of reasons as to why a the development of a new piece of software can end abruptly and/or before it is brought to the market, such as, for instance, it may be being developed by a post-doctoral student who leaves the development team.

Within EMMC we are working to understand how academic software developments can be better supported in order avoid problems such as this and thus to help practically support developments to the market in a more timely manner. A part of this involves making the documents that we generate from the meetings we hold on areas such as different methods of professional software development or software licensing aimed at academic developers publicly available via our website.



The EMMC is working to bring the exploitation of materials modelling to industry and so speed up the lab-to-market process

Industry has also highlighted what it perceives as a lack of communication as one of the reasons why some useful models are not being used to the extent that we would like to see. According to this argument, knowledge is not flowing between different modelling communities. Indeed, in many instances we have seen that different applications sectors actually encounter similar problems, and they could therefore benefit from more synergy in the use of different models.

While this may seem to paint a somewhat negative picture, however, it should be highlighted that there are also some good examples of where things are working well.

Could more be done to incorporate modelling into the engineering/design element, as well as perhaps into company's decision-making process?

Today, in most instances at least, materials modelling is undertaken within the R&D departments of companies, where they focus their activities on gaining a better understanding of physical phenomena or on figuring out why things do not work. However, we are now indeed beginning to see the integration of modelling into engineering and design.

Very often, small companies do lack some of the necessary skills for modelling, which is a problem. As such, there is a need for them to employ experts known as 'translators', who have the expertise to be able to transfer industrial problems into cases to be simulated. This is something we would like to help companies achieve, and, again, we have made documents and guidelines around this subject publicly available on our website.

With regard to these challenges and the barriers to a wider roll out, especially when it comes to SMEs, what do you feel are the biggest benefits and challenges of ICME approaches?

The biggest benefit would be its ability to foster materials innovation and thus make the companies more competitive on the market. In addition, it would also enable them to gain a better understand with regard to processing, properties, and characterisation, from chemistry to application performance. This will subsequently cut costs and time by avoiding unnecessary experiments or perhaps the usage of expensive and dangerous materials.

The screening of a material's properties of materials would reduce the time to market as it helps to solve some very specific problems which perhaps cannot be analysed via experiments.

In that sense, could ICME be one of the ways to overcome the issue of cost which has been cited by industry as one of the main barriers to the wider use of modelling – if, of course, the data is available to demonstrate its potential?

Yes, absolutely. We have worked quite extensively on the economic impact of materials modelling with regard to return on investment with industrial players, and they presented some case studies to demonstrate how it has enabled them to have a shorter time to market as well as higher margin products. However, these tools must have a high level of accuracy and also be application-oriented (as opposed to only being material-oriented) for them to be taken up by industry.

There are currently two European projects – which were initiated within the EMMC roadmap and later funded by the European Commission – on business decision support systems and the development of tools which, besides materials modelling and the technical development of materials, will also incorporate other business-related aspects which will help to support industry's decision making process.

Industry has informed us that it is important to collect the success stories from large companies and small companies alike and to present the measurable benefits of modelling. This kind of dissemination is indeed crucial because it demonstrates to other companies that there are economic benefits to be gained through the incorporation of modelling in certain application fields, and this will go on to support their acceptance and exploitation by others. However, this can be quite difficult to achieve as much of the data on this topic is confidential data, and it can take a long time to get approval from companies to publish it.

At the EMMC we have nevertheless managed to obtain some data of this type and within the next year we hope to have more. We are working with some companies and are trying to further encourage the users to provide quantitative estimation indicators regarding the economic benefits of modelling which we are able to communicate to the field in order to support a wider exploitation of these tools. We had also hoped to collect negative case studies, but as people tend not to want to talk about things that have not been successful we have decided to abandon that.

Software development takes 10-15 years before marketable software tools emerge

Multidisciplinarity is a key element of ICME. Do you feel more could be done in a wider sense to bring together materials and computational mechanics scientists, mathematicians and technologists?

ICME and materials modelling in a very general sense could definitely benefit from a more interdisciplinary approach. Indeed, those working in the field can have very different areas of expertise, and so we now need to enhance the networking that is taking place in order to foster a better exchange between the different stakeholders. This is a trend we are seeing in other fields, but materials modelling seems to be lagging behind.

One way this can be achieved is through the establishment of a 'one stop shop' – essentially a marketplace or innovation hub where all those who offer the services, who use the services, who offer the tools or models, or the translators are able to meet and exchange ideas or find data or documents. In this area, two European Commission-funded projects, which began in January 2018, are currently running in the field of materials modelling. A common platform such as this will allow the data and knowledge to be managed effectively, whilst also allowing the infrastructure and databases to all become connected.

Are there issues with regard intercompatibility of models or data?

Some industrial problems can be very complex and cannot be solved with one existing model – or perhaps the existing model is not adequate. As such, it can be necessary to link or couple models or tools. This requires a consideration on the interoperability between models and experimental and numerical simulations and how they can be integrated together in a single useful workflow for a specific industrial application.

Currently, however, there is a lack of interoperability and standardisation, and this is something we are working to address in the EMMC in order to support the transfer of data and knowledge from one scale to another, or from one model to another, and to establish standardised ways to manage the data. This is taking place on the level of exchange between models or tools or even how to document the data to make it interoperable between different repositories so that it can be used between communities as data repositories can talk to each other and exchange information.

What would you say are the most important points in the EMMC's Vision Beyond H2020?

We would like to see different actions in place to bring European materials modelling marketplaces, open translation environment testbeds, and innovation platforms, which also include characterisation, forwards towards a large scale infrastructure such as that found for HPC so as to enable one true single digital marketplace for innovation in Europe.

Our vision for the future of materials modelling sees the need for this field to be integrated within the higher level trends in industry, such as digitalisation and within Industry 4.0 with new business models based on the integration of models and products. Materials modelling needs to be tightly integrated into emerging informatics systems too so as to become a data source and therefore contribute to delivering on the promises of AI applications in R&D. Similarly, it should also be very tightly connected also experimentation, characterisation, and machine learning. Materials modelling is not something which should stand alone; there is needed synergy with many other disciplines. It is also extremely important for this to be recognised at the European level.

There are a lot of activities taking place to address the interoperability issues due to the fact that the integration of models in product lifecycle management requires joined up information frameworks and ontology development. As such, materials modelling needs to be linked to many other areas in order to enable all stakeholders to build a system and communicate on a shared semantic basis.

The marketplace or innovation hubs mentioned earlier demonstrate that there is progress being made towards a higher level of synergy, and I believe we will see much more of this in the coming years as we will need numerous actions in order to generate new content and to link the existing content into the emerging marketplaces. And, of course, everything should have a common reference standard in order to have an easy integration in the marketplace.

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