Materials Modelling and Digitalisation: a core technology in a post-COVID world

Statement by the European Materials Modelling Council

EMMC ASBL

The European Materials Modelling Council

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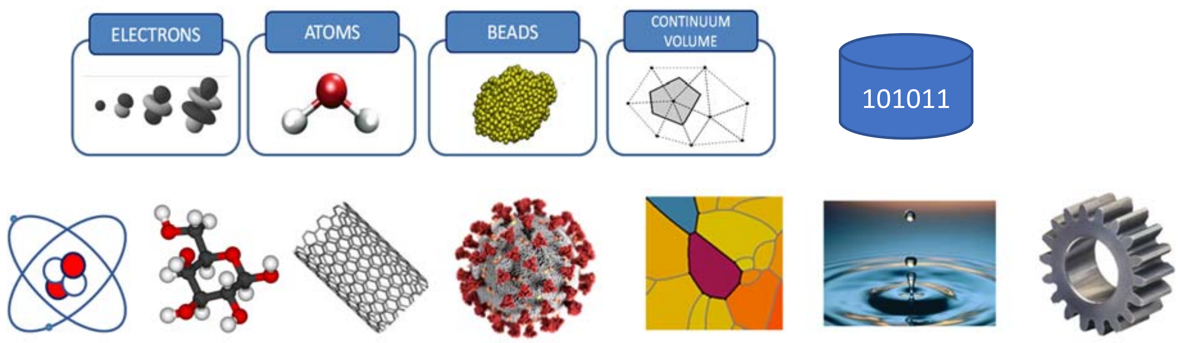
The COVID pandemic has highlighted and amplified shortcomings as well as strengths of modern society: its vulnerabilities to disruption of a world with global interactions and supply chains on the one hand and its ability to adapt quickly and offer solutions in response to the challenge on the other hand. Our way of working had to change as a result and there are likely to be long lasting transformations ahead. The pandemic has also reinforced the urgency and desire to address sustainability challenges and put even greater emphasis on the actions outlined e.g. in the European Green Deal.

These developments are set to continue. The longer society is subject to pandemic control measures, the more digitalisation is expected to grow, and the more important digitalisation will become for companies and society[1]. Both individuals and organisations have come to realise the benefits and opportunities of a more digitally connected and digitally driven world, reducing the need to physical travel, saving time and resource on commuting and in many cases the ability to carry out substantial work for example in R&D by means of a computational, model-based approach.

In all of these aspects, materials and our ability to understand and utilise their behaviour play a central role. Below, we elaborate some key points that underline the strategic importance of materials modelling[2] and digitalisation as key enablers of solutions to societal challenges in European post-COVID society.

What is Materials Modelling?

Materials modelling[2] covers the material behaviour and properties of any type of matter at any scale, from atoms and molecules and nanoparticles to macroscopic objects. Modelling is done by physics-based (electronic, atomistic, mesoscopic, continuum) and data-based models.



1. **Materials modelling for understanding and predicting the (COVID-19) virus behaviour**

   To support science-based decision making, a fundamental understanding of materials behaviour is needed. This level of understanding and in particular the ability to make decisions that affect our lives requires sound materials models; models that are able to reliably and accurately predict the behaviour of nano-sized biological materials (e.g. viruses (20-500 nm in size) and small bacteria (around 500 nm)) and deliver answers to "what if.." questions. The debate around the behaviour of SARS-CoV-2 virus (nano) particles in different environments, how far they can travel, on what they adhere better, what surfaces can eliminate them, how they dock on a cell wall, how toxic they are etc., demonstrates a need for complex multi-scale simulations to shed more light on the situation. It highlights the need for both immediate, applied efforts as well as long-term research into modelling of complex material systems, and more reliable, efficient and robust methods & tools.

2. **Materials modelling for development of vaccines and drugs as well medical devices**

   New levels of expectation for research and development timelines and practices have been set as a result of the pandemic experience. The speed of development of anything from medical ventilators and other treatment devices to new vaccines has shown the power of many computational and digital approaches that were brought to bear. It demonstrated the impact of a change from purely physical to more model-based design and development of materials and products that has already taken place over the last decade, with the pandemic highlighted and amplifying its advantages.

   The development of vaccines and drugs is not only a question of biology and clinical testing, but also one of chemistry and materials. Modelling materials and particle stability, polymorphism, solubility and biopharmaceutical behaviour play a big role in ensuring that development times can be kept to a minimum. As exemplified in a recent paper[3], materials modelling also greatly contributed to a so-called material-sparing approach, whereby development programs can be carried out with a minimum available material, a factor that has actually become crucial in the COVID scenario, due to lack of time, lack of lab resources and issues with global supply chains. Furthermore, computational (in-silico) modelling also contributes to reducing the number of animals sacrificed for the experimental models in line with the 3R strategies (Replacement, Reduction and Refinement) endorsed by the European Commission[4].

3. **Materials modelling for the design of antibacterial and antiviral surfaces, coatings and detergents.**

   In an ever crowded, global world, cross contamination and spread of viruses can be very rapid unless drastic measures, such as lockdowns are imposed. Designing surfaces coating and paints that are sustainable and have properties that can attract and eliminate hazardous particles can be very efficient in limiting the propagation. Further research is needed into (1) paints, coatings and surface structuring and (2) models for how such surfaces can limit the spread and (3) molecular level engineering combined with system engineering on how to position the surfaces optimally. Creating self-cleaning surfaces would be a likely by-product with an impact on energy saving.

New and improved formulations e.g. washing liquids today are already developed largely without physical testing. All relevant properties are determined by modelling, making the process much more agile. Digital twins provide the status of production lines without physical presence. New drugs can be developed with much reduced need to valuable chemicals, higher confidence and greater speed. Further investment into materials modelling and digitalisation will provide organisation with a significant competitive advantage and a much reduced risk profile to potential future pandemic disruptions.

4. **Digital working: maintaining productivity in a safe manner, while reducing the burden of commuting**

In times of confinement and social distancing, our technological ability to support digital working means that organisations and their staff have been able to keep going in a productive and safe manner[5]. In the materials and engineering sectors, digitalisation of plant and operations have enabled a growing number of materials engineers and their colleagues to work virtually from a remote location, thus keeping their company up and running and productive, while preserving the safety of the workforce as well as their respective households. In fact, in many cases, companies experienced an increase in productivity, hence work performed from home offices has proven to be highly efficient in keeping up a functioning and productive society, while reducing the environmental burden of commuting.

In order to build further on these gains, we need high quality software and digital deployment, reliable networks, and of course reliable electric energy. Advanced materials and their processing on the nano-scale play a key role in the development of information and communication technology, e.g. materials for high-frequency applications for 5G networks. Materials modelling enables reaching optimal solutions efficiently and fast. Europe has the opportunity to ensure independence and establish leadership in all these areas.

5. **Democratisation of manufacturing and production resilience thanks to digitalisation: Additive Manufacturing**

During the COVID-19 lockdown, the global 'just in time' supply chain has met its limitations across the world. This opens doors for more distributed and democratised manufacturing processes. More and more local industries and consumers experience the benefit and satisfaction of designing and/or manufacturing their own products by means of Additive Manufacturing (AM).

This evolution will be enabled by improved materials modelling to support reliable AM and integrated into software as a service (SaaS) companies in the cloud, offering solutions to optimise the quality of 3D printed products. This will include digital materials design, the design of the product, the virtual assessment and optimisation of the product performance and the design and optimisation of support structures.

The digitalisation of AM will enable accelerated development and creation of medical devices to fight COVID-19 and beyond. This will include designing and creating new ventilators and other devices, but also enable localised 3D printing of replacement parts, hence reducing the societal dependency on the global supply chain of critical parts

6. **Materials modelling ensuring secure, reliable and sustainable energy supplies**

   Materials modelling has been making very significant contributions to improving materials and discovering new materials to enable renewable and sustainable energy supplies. These include wind turbine blades and their lubrication systems that can run for extended period of times in order to make their use in harsh conditions (off shore) viable, as solar materials that have increase conversion and battery materials with higher energy density, while being save and sustainable. It also includes improved catalysts for lower energy, higher efficiency processes as well as reducing the impact of the catalyst materials themselves.

   Finally, reliable primary energy is critical. Existing nuclear infrastructure is often maintained for longer periods and numerical tools are essential to determine safety levels regarding the materials deterioration in existing plants. In future, advanced modular nuclear reactors are likely to take their part and materials modelling plays a key role to create safe and sustainable engineering solutions for these advanced designs.

7. **Modelling and digitalisation supporting a circular economy**

   A sustainable and circular economy relies on making the best of the valuable materials resources we have. That means optimising their use which in turn means deep understanding and multi-disciplinary optimisation based on sound models. It also means providing a digital record for each material in each product that tells users and machines how to use, maintain and re-use the materials, an approach that requires models to be passed along with the materials.

8. **Materials modelling enabling cross-disciplinary research**

   Materials modelling stretches across all scales and is inherently inter-disciplinary. During the COVID crisis, there have been increased cross-disciplinary interactions between life science and materials modelling; many materials modelling groups have now started to work with biotechnology-related problems. The experience and competence arising from these interactions will not only benefit the handling of the current COVID situation, but also facilitate involving materials modelling in other biology-related challenges, with great impact potential.

In conclusion, materials modelling and digitalisation is invaluable in our mission to solve the pressing challenges as well as realising the opportunities of a post-COVID society.

Europe is in a leading position in all of the above points, i.e. in fundamental and applied materials science, in academic development of modelling and digitalisation as well as in commercial software, Europe being the home of some of the largest as well as most innovative companies in the field.

The European Materials Modelling Council brings together all relevant stakeholders and calls on policy makers, grant bodies and industries to support materials modelling and digitalisation investments for a more sustainable and resilient European society.

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