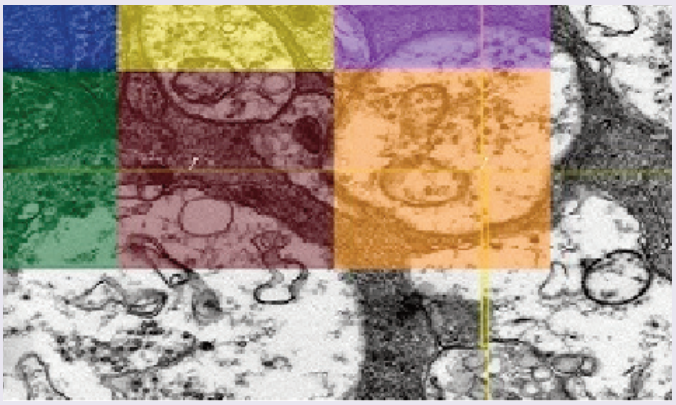
CASE STUDY

Newton Gateway to Mathematics

Predictive Multiscale Materials Modelling

BACKGROUND



The multiscale/ multiphysics nature of materials gives rise to extremely challenging and unique mathematical and algorithmic problems currently prohibiting uncertainty quantification and predictive materials modelling. The ability to predict the properties of these materials with confidence is paramount to a number of sectors.

The Gateway delivered a four day research workshop in December 2015, in collaboration with and supported by the Warwick Centre for Predictive Modelling (WCPM) and the Knowledge Transfer Network (KTN), to introduce and debate interdisciplinary approaches for addressing bottlenecks in predictive materials modelling. Currently there is a huge gap between state-of-the-art mathematical methods and the analysis and computational tools routinely used by the materials community. Additionally, in the context of the revolution that is taking place in the data sciences, the workshop focused on the development and exploration of data-driven models of material systems that effectively integrate available data from simulations and experiments with physical models towards predictive multiscale materials modelling.

CHALLENGES

The workshop aimed to identify the gaps in the tools and methods used in predictive multiscale materials modelling and propose some solutions and collaborative opportunities to address these. One major scientific challenge for instance was to identify needed advances in fundamental mathematical, statistical and machine learning approaches to impact data-driven predictive multiscale materials modelling and design.

From an industry perspective, it is recognised that many sectors stand to benefit from mathematical innovations which lead to rapid materials development and deployment. Fundamental problems such as the need to improve the timeliness and cost-effectiveness of materials engineering processes for new designs and design changes are well known. There is a need to replace today's experimentally-based qualification processes with more effective modelling and probabilistically-based materials engineering.

There are a key number of modelling challenges to be addressed, including:

- Devising methods and protocols for addressing rare events and extreme value statistics;
- Modelling across different but coupled time and length scales;
- Developing probabilistic hierarchical and multiscale models;
- Exploring high-dimensional structure/property/process relations.

The workshop provided an ideal environment not possible elsewhere for bringing together national and international leading academics and industrial researchers, to address and debate interdisciplinary solutions to unifying mathematical themes fundamental to predictive materials modelling. The different perspectives presented and the opportunity to discuss mathematical and statistical challenges arising in predictive materials modelling in industrial applications have contributed to a long lasting impact"

PROF. DR. NICHOLAS ZABARAS
DIRECTOR, WARWICK CENTRE FOR PREDICTIVE MODELLING

ACTIVITY

To help identify advances, the workshop brought together perspectives from nearly 100 national and international leading scientists, as well as delegates from industry and the public sector, who could benefit from mathematical innovations. It involved those in computational materials, physics, chemistry, uncertainty quantification and machine learning, as well as those in the aerospace, pharmaceutical, electronic, automotive and energy industries.

Talks presented perspectives from both academia and industry, and there were a number of facilitated industry led open panel discussions sessions, with input from NPL, Airbus and Dassault Systèmes : BIOVIA. These included *Predictive Materials Modelling in the Energy Sector, Predictive Materials Modelling in the Aerospace and High Value Manufacturing Sectors and Predictive Materials Design and Discovery.*

IMPACTS

The industry led panels discussed both predictability challenges that the materials industry faces, but also the value of integrating recent academic advances in predictive modelling to industrial practices. The impact of adopting new approaches in the materials industry is significant, as it may lead to virtual certification of materials and products, accelerated insertion of new materials in industrial applications, design of materials with unprecedented (extremal) properties leading to new products and applications & prognosis of future failure and performance of devices and products using historical data.

> ***"I was very pleased to finally meet people from engineering, mathematics, chemistry, physics departments in the UK in one place and exchange ideas with them."***
>
> PARTICIPANT

The methods discussed in the workshop have significant potential to reduce the cost, time and risk of material system validation for advanced materials, assessment of new design configurations at the component level, and for assessing risk and capability at the system level.

Some key conclusions reached over the course of the workshop were:

- Mathematical and statistical developments for data-driven approaches to predictive materials modelling are of paramount importance for the accelerated design of materials and processes in the presence of inherent structure, process, model and epistemic uncertainties.
- The importance of the identification and integration of synergistic methodologies from different research fields (including materials physics and chemistry, uncertainty quantification, machine learning and optimisation) towards predictive materials modelling.
- Machine learning approaches can be used to predict materials properties or to distil large amounts of complex data into a comprehensive form.

> ***"For me it was good to understand where academia is, and where we can use them. I had some good discussions and made some good contacts. I hope I can return and do an update on where we are in predictive analysis."***
>
> PARTICIPANT

A highlight of the workshop was the poster exhibition which offered participants the opportunity to display information related to their work or area of research.

A special edition of the Journal of Computational Physics was published in Autumn 2016 and included submissions of research and review papers related to the focus of the workshop. This is a premier journal in computational sciences, uncertainty quantification and multiscale modelling research.

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